

## Operator separation of variables for adiabatic problems in quantum and wave mechanics

V. V. BELOV<sup>1</sup>, S. YU. DOBROKHOTOV<sup>2</sup>, and T. YA. TUDOROVSKIY<sup>2</sup>

<sup>1</sup>*Institute for Electronics and Mathematics, Trekhsvyatitelskiy per., 3/12, 109028 Moscow, Russia*  
(e-mail: [belov@miem.edu.ru](mailto:belov@miem.edu.ru))

<sup>2</sup>*Institute for Problems in Mechanics Russian Academy of Sciences, prosp. Vernadskogo, 101-1, Moscow 119526, Russia* (e-mails: [dobr@ipmnet.ru](mailto:dobr@ipmnet.ru); [timtudor@mail.ru](mailto:timtudor@mail.ru))

Received 26 July 2004; accepted in revised form 28 February 2006 / Published online: 25 July 2006

**Abstract.** Linear problems in mathematical physics where the adiabatic approximation is used in a wide sense are studied. From the idea that all these problems can be treated as problems with an operator-valued symbol, a general regular scheme of adiabatic approximation based on operator methods is proposed. This scheme is a generalization of the Born–Oppenheimer and Maslov methods, the Peierls substitution, etc. The approach proposed in this paper allows one to obtain “effective” reduced equations for a wide class of states inside terms (*i.e.*, inside modes, subbands of dimensional quantization, etc.) with possible degeneration taken into account. Next, by application of asymptotic methods, in particular the semiclassical approximation method, to the reduced equation, the states corresponding to a distinguished term (effective Hamiltonian) can be classified. It is shown that the adiabatic effective Hamiltonian and the semiclassical Hamiltonian can be different, which results in the appearance of “nonstandard characteristics” while passing to classical mechanics. This approach is used to construct solutions of several problems in wave and quantum mechanics, particularly problems in molecular physics, solid-state physics, nanophysics and hydrodynamics.

**Key words:** adiabatic and semiclassical approximation, Born–Oppenheimer method, electron-phonon interaction, interval waves, Maslov operator methods, nanofilms, picnocline

### 1. Introduction

Many linear problems in mathematical and theoretical physics contain different spatio-temporal scales. Among them there are problems in molecular physics, problems concerning electron waves in crystals, wave propagation in media with rapidly varying characteristics, surface and internal waves in fluids, electron-phonon interaction, electromagnetic waves and quantum particles propagating in waveguides, etc. The main instruments for investigating such problems are contained in the adiabatic approximation, which is based on the idea of separating “fast” and “slow” modes by means of “freezing” the slowly varying variables. For instance, the “slow” variables describe the nuclear motion in molecules and the “fast” variables concern the electron motion, or the “slow” variables describe the longitudinal motion and the “fast” variables describe the transverse motion in thin waveguides. Needless to say that there are many different versions of adiabatic approximation and thousands of papers and monographs related to this approach and its applications in different fields of mechanics and physics. Among these we mention [1–10]. Nevertheless, we take the liberty to present a general regular scheme of the adiabatic approximation suggested in [11–13] and combine different approaches including the Born–Oppenheimer method, the Maslov operator method, the Peierls substitution, etc. From a mathematical point of view, the equations (or the system of equations) describing all these phenomena have the same structure. Namely, following [6], these equations (systems) can be

treated as equations with an “operator-valued symbol.” Our idea to study such equations is not new: the asymptotic analysis of the original problem can be divided into two parts: (1) the “operator” reduction to simpler differential or pseudodifferential equations with the principal symbol, known in different fields of physics as an effective Hamiltonian, or term, or dispersion relation, or mode, etc., and with corrections to this symbol; (2) asymptotic constructions of the solutions of this simpler reduced equation based on different variants of the semiclassical approaches, like the WKB-method, Born approximation, oscillatory approximations, ray expansions, the Maslov canonical operator, averaging, etc. Here we present the first part of this concept in the form of a regular rigorous algorithm (in Section 3), based on operator methods [14].

The result of the first step is the reduced equation; it has different names in different fields of physics; we call it the *effective equation of adiabatic motion*. We illustrate the “operator” reduction or the “operator separation” of variables by using the above-mentioned problems from different fields of physics and, in Section 4, present the corresponding equations for the wave functions of adiabatic motion. The examples given in Sections 4.1–4.4 were studied long ago, whereas the results of Sections 4.5–4.6 (as well as Section 5) were obtained by the authors recently.

To realize the second step, it is necessary to take into account that usually the original problem includes several parameters. Some of these, like the transverse and longitudinal characteristic sizes of a waveguide or the ratio between the masses of light and heavy particles, allow one to use the adiabatic approximation and do not crucially correlate with the energy of adiabatic motion. Other parameters, like the magnitudes of the external electromagnetic field, the momentum of the incoming wave in the scattering problem, etc., determine the energy. This fact implies different forms of (asymptotic) wave functions of adiabatic motion and, as a consequence, a redefinition of the principal symbol and the effective Hamiltonians depending on the relations between the above-mentioned parameters. In turn, it gives different types of characteristics (trajectories of Hamiltonian systems) which Maslov [15] called “nonstandard characteristics” and which must be used in asymptotic constructions. We discuss the possible classification of these characteristics using, as the main example, the quantum-wave propagation in thin (or *nano*) tubes. In spite of the fact that the given arguments seem to be natural, and in some way appear in the physical literature, they do not seem to have been applied systematically. The methods for constructing asymptotic or exact solutions of the “redefined” equation for the wave functions of adiabatic motion are well known and here the results must be connected with a concrete physical problem. Therefore, we do not construct asymptotic solutions for most of the derived reduced equations and in Section 5 only briefly describe different solutions for the equations of quantum particles in nanostructures.

The main results of the “operator separation of variables” are realized in Equations (3.5), (3.7) and (3.11). Although they simply follow the Born–Oppenheimer approach or those of Peierls and Maslov, nevertheless they allow us to consider a wide range of adiabatic problems uniformly and in a rather compact form. We believe that this approach is very useful in different situations, since it gives not only a general regular scheme for deriving the reduced equations exactly but allows one to obtain qualitative and quantitative estimates of the range of applicability of any approximation. Naturally, the argument resulting in Equations (3.5) and (3.7), the classification of different approximations, the relations between the adiabatic and semiclassical asymptotics, etc. can be better illustrated with a simple example. These considerations, some of which are well known in physics and some of which are well known in mathematics, are given in Section 2 and Sections 3.1–3.2. In Section 2, we present a minimal amount of the required information from the operator calculus of noncommuting operators

[14] (see also [16]). We point out that the facts from [14] used here are not simply arguments of the “mathematical justification and verification” type, but are completely constructive and developed algorithms that are well adjusted to the problems studied here.

Finally we can formulate the main result of the paper as follows. We suggest the regular asymptotic (adiabatic) procedure which allows one, (1) to determine correctly the leading part of asymptotic solution corresponding to wide diapason of energies (or frequencies), (2) to construct and estimate if necessary the “adiabatic” corrections. Needless to say that in this work we understand an asymptotic solution in the formal sense, *i.e.*, in the sense of small “right-hand side” (discrepancy). The proof of the fact that the constructed asymptotic solution approximates some exact solution of the original equation is outside the scope of the present study and we will touch upon this problem only very briefly.

**2. Differential and pseudodifferential operators with a parameter and their symbols.**

**Elementary formulas from calculus of noncommuting operators**

We want to study some asymptotic solutions of (systems of) partial differential equations with small parameter  $\mu$  in the configuration space with coordinates  $x = (x_1, \dots, x_N)$  which can be written in general form:

$$i\Psi_t = \hat{\mathcal{H}}\Psi. \tag{2.1}$$

Here  $\Psi(x, t)$  can be a scalar or vector function,  $\mathcal{H}$  is a partial differential scalar or matrix operator. It is convenient for us to present the operator  $\mathcal{H}$  as a function of noncommuting operators  $-i\partial/\partial x = (-i\partial/\partial x_1, \dots, -i\partial/\partial x_N)$  and  $x = (x_1, \dots, x_N)$  and, generally speaking, of time  $t$ :  $\hat{\mathcal{H}} = \mathcal{H}(-i\partial/\partial x_1, \dots, -i\partial/\partial x_N, x_1, \dots, x_N, t)$ , where the function  $\mathcal{H}(p_1, \dots, p_n, x_1, \dots, x_N, t)$  is usually called the symbol of the operator  $\hat{\mathcal{H}}$ . Actually, we shall consider the situation in which the function  $\mathcal{H}$  can depend on the parameter  $\mu$  and also on some other ones. Quite often a small parameter  $\mu$  appears as a factor before the derivatives  $\partial/\partial x_j$ , say, before  $\partial/\partial x_1, \dots, \partial/\partial x_n, n \leq N$ . It follows from the considerations given below that there is always a parameter  $\mu$  before  $\partial/\partial t$ . We denote the other variables by  $y_1, \dots, y_m, m = N - n$ . So finally Equation (2.1) takes the form

$$i\mu\Psi_t = \mathcal{H}\left(-i\mu\frac{\partial}{\partial x_1}, \dots, -i\mu\frac{\partial}{\partial x_n}, x_1, \dots, x_n, -i\frac{\partial}{\partial y_1}, \dots, -i\frac{\partial}{\partial y_m}, y_1, \dots, y_m, t, \mu\right)\Psi. \tag{2.2}$$

As the operators  $\partial/\partial x_j$  and  $x_j$ , as well as operators  $\partial/\partial y_k$  and  $y_k$  do not commute, one has to agree about the order of action of  $x_j$  and  $\partial/\partial x_j$  and, analogously, of  $y_k$  and  $\partial/\partial y_k$ . The theory of functions of noncommuting operators is very well developed [14]; see also [16–18]. For the sake of completeness, let us present a minimal amount of the required information from operator calculus and recall the terminology.

First, let  $R(x, p) = \sum_{k=0}^l R_k(x)p^k$  be a polynomial in variables  $p$  with coefficients that are smooth in  $x$ . This function generates the operator  $\hat{R} = \sum_{k=0}^l R_k(x)(-i\mu\frac{\partial}{\partial x})^k$ . The function  $R(x, p)$  is called the symbol of the differential operator  $\hat{R}$  with a parameter  $\mu$ . It is clear that the way of constructing the operator  $\hat{R}$  by means of the symbol  $R$  is not unique. For example, one can build an operator  $\hat{R}' = \sum_{k=0}^l (-i\mu\frac{\partial}{\partial x})^k R_k(x)$ , different from  $\hat{R}$ . Using the Feynman notation, we can write  $\hat{R} = R(\hat{p}, \overset{1}{x})$  and  $\hat{R}' = R(\hat{p}, \overset{2}{x})$ , where the numbers above  $\hat{p}$  and  $x$  determine the order of their action. (About other ways of ordering, for instance, by Weyl, see [14]). In this work, we will always use the first way of ordering. Under this agreement,

the definition of the differential operator is equivalent to the definition of its symbol. By letting the order of the polynomial  $k$  tend to infinity, one can obtain, at least, “naive” operators whose symbols are not polynomials. Such operators are called pseudodifferential. Their rigorous definition is given by means of the “ $\mu$ -Fourier transform” [6, 14]:

$$A(\hat{p}, \hat{x})\varphi(x) = F_{p \rightarrow x}^\mu [A(p, x) [F_{x \rightarrow p}^\mu \varphi(x)](p)](x); \tag{2.3}$$

here the direct and inverse “ $\mu$ -Fourier transforms”  $F_{x \rightarrow p}^\mu$  and  $F_{p \rightarrow x}^\mu$  are defined by the equalities:

$$[F_{x \rightarrow p}^\mu \varphi(x)](p) = \frac{1}{(2\pi i\mu)^{n/2}} \int_{\mathbb{R}^n} e^{-i(p,x)/\mu} \varphi(x) dx,$$

$$[F_{p \rightarrow x}^\mu \tilde{\varphi}(p)](x) = \frac{1}{(-2\pi i\mu)^{n/2}} \int_{\mathbb{R}^n} e^{i(p,x)/\mu} \tilde{\varphi}(p) dp.$$

From now on,  $\langle , \rangle$  is the inner product in the Euclidean space of the corresponding dimension.

The replacement of operators by their symbols turns out to be very useful in practical calculations. As a result, the calculations concerning operators are replaced by significantly simpler work (which can be algorithmized) with symbols, *i.e.*, functions (“with  $c$ -numbers”). Since, in asymptotic approaches, defining an operator is practically equivalent to defining its symbol, in the process of obtaining asymptotic formulas *one can manipulate only with symbols and “recall” the operators corresponding to these symbols only in studying refined problems such as, for example, justification of the asymptotic accuracy of the solutions constructed.* Of course, the main difficulties in dealing with functions of operators arise due to the fact that the operators  $\hat{p}$  and  $x$  do not commute. On the other hand, their commutator is  $i\mu$ , and it is small, which allows one to use asymptotic expansions in the constructions. In view of this fact, it is natural to consider the symbols  $R$  depending on the parameter  $\mu$  and to assume that  $R(p, x, \mu) = R_0(p, x) + \mu R_1(p, x) + \dots$ . Moreover, the right-hand side in this relation is understood as an asymptotic expansion in the parameter  $\mu$ . The function  $R_0(p, x)$  is called the leading symbol or, sometimes, a Hamiltonian, and  $R_j$  are called  $j$ th-order corrections.

The next generalization consists in the assumption that the symbol of the operator  $\hat{R}$  may be *an operator*. A simple example appears in the situation in which  $R(p, x, \mu)$  is a matrix (or an operator acting in a finite-dimensional space).

2.1. EXAMPLE 1. THE KLEIN–GORDON EQUATION

Consider, for instance, the Klein–Gordon equation  $\mu^2 \varphi_{tt} - \mu^2 \varphi_{xx} + v(x)\varphi = 0$  written in vector form for the vector function  $\Psi = \begin{pmatrix} \Psi_1 \\ \Psi_2 \end{pmatrix} = \begin{pmatrix} \varphi \\ \varphi_t \end{pmatrix}$ :

$$i\mu \Psi_t = \mathcal{H}(-i\mu \partial / \partial x, x) \Psi, \quad \Leftrightarrow \quad \begin{cases} i\mu \Psi_{1t} = \Psi_2, \\ i\mu \Psi_{2t} = v(x)\Psi_1 - \mu^2 \Psi_{1xx}. \end{cases} \tag{2.4}$$

The symbol of the operator  $\mathcal{H}(p, x)$  is the  $2 \times 2$  matrix function

$$\mathcal{H}(p, x) = \begin{pmatrix} 0 & 1 \\ p^2 + v(x) & 0 \end{pmatrix}.$$

From this viewpoint, one can consider many fundamental physical equations like the Dirac and Pauli equations, the Lamé equation in linear elasticity theory, the linearized equations of hydrodynamics, etc. (If they include a small parameter in an appropriate way.) The

appearance of a small parameter  $\mu$  before the derivative  $\partial/\partial x$  is very important in our constructions. As we have mentioned, there exist many problems with different scales in which a small parameter appears only in front of some derivatives. Problems of such types give the majority of nontrivial  $\mu$ -differential operators with operator-valued symbols.

## 2.2. EXAMPLE 2. MOLECULAR PHYSICS

Consider, for instance, the Schrödinger equation for two groups of particles: heavy atomic nuclei with mass  $M$  and light electrons with mass  $m$ . We denote the coordinates of nuclei and electrons by  $x'$  and  $y'$ , respectively. Let us assume that  $l_0$  is the linear size of a molecule and  $d_0$  is the amplitude of nuclear oscillations. Thus, the characteristic magnitude of the electron energy is  $\varepsilon_e \sim \hbar^2/(2ml_0^2)$ . For physical reasons (stated by Born and Oppenheimer), the motion of a nucleus could be considered in the oscillatory approximation and its energy is  $\varepsilon_n \sim \hbar^2/(2Md_0^2) \sim kd_0^2/2$  with the elasticity coefficient  $k$ . To estimate  $k$ , one has to remember that, in the adiabatic approximation, the potential energy of a nucleus is the total energy of electrons [19], so  $k \sim \partial^2 \varepsilon_e / \partial x^2 \sim \hbar^2/(ml_0^4)$ . Thus we have  $\hbar^2/(2Md_0^2) \sim \hbar^2 d_0^2/(2ml_0^4)$ . From this, we obtain  $d_0/l_0 \sim (m/M)^{1/4}$ . Oscillatory energies of nuclei and electrons relate as  $\varepsilon_n/\varepsilon_e \sim (m/M)(l_0^2/d_0^2) \sim (m/M)^{1/2}$ . Let us introduce the parameter  $\mu = (m/M)^{1/2}$  and divide both sides of the Schrödinger equation by  $\hbar^2/(2ml_0^2)$ . After passage to dimensionless variables  $x = x'/l_0$ ,  $y = y'/l_0$ , the stationary Schrödinger equation takes the form

$$\hat{\mathcal{H}}\Psi = E\Psi, \quad \hat{\mathcal{H}} = \left( -\frac{1}{2}\mu^2\Delta_x - \frac{1}{2}\Delta_y + v(x, y) \right): \quad (2.5)$$

The symbol  $\mathcal{H}$  of the  $\mu$ -differential<sup>1</sup> operator  $\hat{\mathcal{H}}$  is again the operator

$$\mathcal{H}(p, x) = \frac{1}{2}p^2 - \frac{1}{2}\Delta_y + v(x, y). \quad (2.6)$$

Usually,  $x$  are called *slow variables* and  $y$  are called *fast ones*. Close approaches to the determination of electron states (*terms*) in a molecule can be found in [6, 8, 9, 20].

## 2.3. EXAMPLE 3. QUANTUM 2-D WAVEGUIDE

One encounters an equation with closed structure by considering a “narrow” straight quantum waveguide. The word “narrow” means that the characteristic width of the waveguide  $d_0$  is much smaller than its length  $l_0$ . We introduce the small parameter  $\mu = d_0/l_0$ . The dynamics of a spinless quantum (quasi)particle in a plane waveguide is determined by the 2-D Schrödinger equation with the potential  $v = v(x, y)$  inside the waveguide. Due to two different scales, there appear two different characteristic energies: the characteristic energy of the lower transverse levels (which is usually called the characteristic energy of the “transverse quantization”) and the characteristic longitudinal energy  $\varepsilon_{\parallel}$ . One can estimate  $\varepsilon_{\perp}$  from the uncertainty principle, which gives  $\varepsilon_{\perp} = \hbar^2/(2md_0^2)$ . Let us introduce dimensionless variables  $x' = x/l_0$ ,  $y' = y/d_0$ ,  $t = (\mu\omega_{\perp})^{-1}$ ,  $\omega_{\perp} = \varepsilon_{\perp}/\hbar$  and dimensionless potentials  $v' = v/\varepsilon_{\perp}$ . Then the corresponding Schrödinger equation takes the form (we omit the primes of the dimensionless variables):

$$i\mu \frac{\partial \Psi}{\partial t} = \hat{\mathcal{H}}\Psi, \quad \hat{\mathcal{H}} = \left( -\frac{\mu^2}{2} \frac{\partial^2}{\partial x^2} - \frac{1}{2} \frac{\partial^2}{\partial y^2} + v(x, y) \right) \Psi. \quad (2.7)$$

The symbol of the  $\mu$ -differential operator is the operator (2.6) with  $\Delta_y = \partial^2/\partial y^2$ .

<sup>1</sup>Born and Oppenheimer in their famous paper [1] used the parameter  $\varkappa = \sqrt{\mu}$ , which is the ratio  $d_0/l_0 \sim \varkappa$  of the characteristic wavelength to the wave function and the linear size of the molecule.

Generalizations of the plane quantum waveguide are quantum thin tubes (nanotubes) and thin films (nanofilms), and their symbols are matrix-operators if one includes spin into consideration. These more complicated examples, as well as several examples from other fields, will be considered later.

Let us again stress that the *definition of the symbol of a  $\mu$ -differential operator differs from the standard definition of the symbol of an operator without parameter*. Namely, we construct the symbol, taking only the slow variables into account. This is why the symbols of the  $\mu$ -differential operator  $\hat{\mathcal{H}}$  in Examples 2 and 3 are again differential operators acting in some appropriate Hilbert space with coordinates  $y$ . The transition to  $\mu$ -differential symbols is a formalization of the idea of “freezing the slow variables.” We discuss the related problems later. The introduction of a small parameter  $\mu$  formally ensures that the commutator  $[x, \hat{\mathcal{H}}]$  is small. There is no universal interpretation of this fact; this depends on each concrete physical problem.

Let us also note that one can consider the equations from Examples 2 and 3 as infinite vector ones. To show this, let us assume, for simplicity, that, for each  $x \in \mathbb{R}^n$ , the spectrum of the operator  $-(1/2)\partial^2/\partial y^2 + v(x, y)$  is discrete and simple and that the corresponding eigenfunctions  $\{w_n(x, y)\}$  and eigenvalues  $\lambda_n(x)$  depend smoothly on  $x$ . Then one can expand any solution  $\Psi(x, y, t)$  of Equation (2.7) in the Fourier series

$$\Psi = \sum_k w_k(x, y)\psi_k(x, t). \tag{2.8}$$

Substituting solution (2.8) in Equation (2.7), we obtain:

$$i\mu \frac{\partial \psi_k}{\partial t} = -\frac{\mu^2}{2} \frac{\partial^2 \psi_k}{\partial x^2} - \mu^2 \sum_n \left\langle w_k, \frac{\partial w_n}{\partial x} \right\rangle_y \frac{\partial \psi_n}{\partial x} - \frac{\mu^2}{2} \sum_n \left\langle w_k, \frac{\partial^2 w_n}{\partial x^2} \right\rangle_y \psi_n. \tag{2.9}$$

If we introduce the infinite vector  $\psi = (\psi_1, \psi_2, \dots)^T$ , then we can represent (2.9) as the following infinite vector equation with infinite-dimensional matrix Hamiltonian  $\hat{\mathcal{H}}$ :

$$i\mu \psi_t = \hat{\mathcal{H}}\psi, \quad \hat{\mathcal{H}} = \mathcal{H}_0(p, x) + \mu \mathcal{H}_1(p, x) + \mu^2 \mathcal{H}_2(p, x),$$

$$(\mathcal{H}_0)_{kn} = \left( \frac{p^2}{2} + \lambda_n(x) \right) \delta_{kn}, \quad (\mathcal{H}_1)_{kn} = -i \left\langle w_k, \frac{\partial w_n}{\partial x} \right\rangle_y p, \quad (\mathcal{H}_2)_{kn} = -\frac{1}{2} \left\langle w_k, \frac{\partial^2 w_n}{\partial x^2} \right\rangle_y.$$

In all examples considered above, the momentum operators corresponding to the slow variables  $x_j$  are  $-i\mu \partial/\partial x_j$ . Of course, one can consider a general situation in which the Hamiltonian depends on the operators  $\hat{x}_j, \hat{p}_j$  generating the Heisenberg algebra with commutators  $[\hat{p}_j, \hat{x}_k] = \mu \delta_{j,k}, \quad \mu \ll 1$ . Such a situation appears in the electron-phonon interaction that we shall discuss in Section 4. The other obvious generalizations of the equations with operator-valued symbols are vector equations containing “slow” and “fast” variables. For instance, we can consider the Pauli equation in a thin quantum waveguide. In this case (see Section 4.6), the symbol is a matrix operator differential with respect to fast variables.

To conclude this section, we present a useful formula which plays an important role in our future considerations. Let  $\hat{A}$  and  $\hat{B}$  be pseudodifferential operators

$$\hat{A} = A(-i\mu \partial/\partial x, \overset{1}{x}, \overset{2}{\mu}), \quad \hat{B} = B(-i\mu \partial/\partial x, \overset{1}{x}, \overset{2}{\mu});$$

then the symbol  $\text{smb}(\hat{A}\hat{B})$  of their product  $\hat{A}\hat{B}$  is equal to (see [14])

$$\text{smb}(\hat{A}\hat{B}) = A(p - i\mu \partial/\partial x, \overset{1}{x}, \overset{2}{\mu})B(p, x, \mu). \tag{2.10}$$

### 3. General scheme of the operator separation of variables in adiabatic problems

#### 3.1. GENERAL STATEMENT OF THE PROBLEM WITH OPERATOR-VALUED SYMBOLS AND PARAMETERS

We are going to construct a certain asymptotic solution  $\Psi = (\Psi^1, \dots, \Psi^s)^T$ ,  $s \geq 2$ , to vector equation (2.2) with a small parameter  $\mu \ll 1$  or its stationary variant

$$\hat{\mathcal{H}}\Psi = E\Psi. \tag{3.1}$$

In (2.2) and in (3.1), the matrix operator (quantum matrix Hamiltonian)  $\hat{\mathcal{H}}$  is generated by its operator-valued symbol

$$\mathcal{H} = \mathcal{H}(p, x, -i\partial/\partial y, y, t, \mu) = \begin{vmatrix} \mathcal{H}_{11} & \dots & \mathcal{H}_{1s} \\ \dots & \dots & \dots \\ \mathcal{H}_{s1} & \dots & \mathcal{H}_{ss} \end{vmatrix},$$

$$\mathcal{H}_{ij} = \mathcal{H}_{ij} \left( p, x, -i\frac{\partial}{\partial y}, y, t, \mu \right), \quad 1 \leq i, j \leq s.$$

(In the stationary case,  $\mathcal{H}_{ij}$  do not depend on time  $t$ .) We assume that the operator-valued symbol (the matrix-operator)  $\mathcal{H} = \|\mathcal{H}_{ij}(p, x, -i\frac{\partial}{\partial y}, y, \mu)\|$  smoothly depends on  $p, x, t$  and acts in an appropriate vector Hilbert space  $\mathbb{H}_y$  with coordinates  $y$  from some domain  $\mathbb{M}_y$  and with the inner product  $\langle \cdot, \cdot \rangle|_y$  (for instance, in  $L_2(\mathbb{M}_y) \times L_2(\mathbb{M}_y) \times \dots \times L_2(\mathbb{M}_y)$ ). Another natural assumption is that the symbol  $\mathcal{H}(p, x, -i\frac{\partial}{\partial y}, y, \mu)$  can be expanded into a regular series with respect to the parameter  $\mu$ :

$$\mathcal{H} \left( p, x, -i\frac{\partial}{\partial y}, y, t, \mu \right) = \mathcal{H}_0 \left( p, x, -i\frac{\partial}{\partial y}, y, t \right) + \mu\mathcal{H}_1 \left( p, x, -i\frac{\partial}{\partial y}, y, t \right) + \dots \tag{3.2}$$

We also assume that the (pseudo)differential operator  $\hat{\mathcal{H}}$  acts in an appropriate expanded Hilbert space  $\mathbb{H}_{x,y}$  with coordinates  $(x, y) \in \mathbb{R}_x^q \times \mathbb{M}_y$  and all the future operations related to them are valid. Of course, one has to verify the last assumption in each concrete problem. Usually (but not always), we shall consider situations in which  $\mathcal{H}$ , as well as the operator  $\hat{\mathcal{H}}$ , are essentially self-adjoint.

It is important to emphasize again that in (2.2) there is a small “adiabatic” parameter  $\mu$  in front of the derivatives with respect to “slow” variables  $x$ , but there is no small parameter in front of the derivatives with respect to “fast” variables  $y$ .

Of course, one has to add additional boundary and initial conditions to Equation (2.2). We shall do this later after the discussion in Section 4, and now we only note that we are going to consider only special problems that are interesting from a physical point of view. The statements of these problems follow the adiabatic separation of the original Equation (2.2) into a set of reduced equations corresponding to different “terms” or “modes” and determined by “effective Hamiltonians” or “dispersion relations.” We present our concept of this separation (the “operator separation of variables”) together with the corresponding formulas in the two subsequent sections.

#### 3.2. ANZATZ OF THE OPERATOR SEPARATION OF VARIABLES

Let us illustrate the main ideas of the operator separation of variables in adiabatic problems with an example of a “quantum waveguide” (2.7). If the potential  $v(x, y)$  is the sum  $v_1(x) + v_2(y)$ , one can separate the variables and find a special solution to Equation (2.7) as a product of two functions (modes)  $\chi(y, \mu)\psi(x, t, \mu)$ . It is clear that this representation is not valid

if  $v(x, y) \neq v_1(x) + v_2(y)$ . Even so, since there are different scales in the longitudinal and transverse directions, we can separate the modes adiabatically. According to the standard adiabatic approach based on the fundamental papers by Born and Oppenheimer, the leading term of the wave function in the adiabatic approximation is sought in the form of the product

$$\Psi(x, y, t, \mu) \approx \chi(x, y, \mu)\psi(x, t, \mu). \quad (3.3)$$

But this representation can be used in a situation when the function  $\psi(x, t, \mu)$  is quite smooth and works poorly for large-enough energies of longitudinal motion. If the function  $\psi(x, t, \mu)$  exhibits fast oscillations, for instance, if  $\psi$  is the WKB-solution  $\psi(x, t, \mu) = \exp(iS(x, t, \mu)/\mu)\varphi(x, t, \mu, h)$ , then representation (3.3) is not convenient for the asymptotic expansion and, instead of formula (3.3), one has to include the classical momentum  $\partial S/\partial x$  into the factor  $\chi(y, x, \mu)$  and use the formula (see [6])

$$\Psi(x, y, t, \mu) \approx \chi(\partial S/\partial x, x, y, \mu)\psi(x, t, \mu). \quad (3.4)$$

Recall that the phase  $S$  is the solution of the Hamilton–Jacobi equation  $\partial S/\partial t + H_{\text{eff}}(\partial S/\partial x, x, t) = 0$  with the so-called effective Hamiltonian  $H_{\text{eff}}(p, x, t)$ . For the case in which  $H_{\text{eff}}(p, x, t)$  is a function of  $p$  only and  $S = -\omega t + px$ , the Hamilton–Jacobi equation is a *dispersion relation*. Formula (3.4) is still not satisfactory, because for the case in which there are focalization effects, *i.e.*, there are turning points or caustics, the WKB-representation is not true, and it is necessary to change the forms of  $\psi$  and  $\chi$ . We propose to “correct” (3.4) in such a way that a new formula would also work in the case of focal and turning points. This correction is based on the observation that, in the WKB-case modulo a small correction, the right-hand side in (3.4) remains the same (see, *e.g.*, [6]) if one assumes that the first factor is the (pseudodifferential) operator  $\chi(-i\mu\partial/\partial x, \overset{1}{x}, y, t, \mu)$  written as a function (its symbol) of the noncommuting operators  $x$  and  $\hat{p} = -i\mu\partial/\partial x$ . Finally, we suggest to look for the solution  $\Psi(x, y, t)$  in the adiabatic approach in the following form [11, 13, 16, 21]:

$$\Psi(x, y, t, \mu) = \chi\left(-i\mu\frac{\partial}{\partial x}, \overset{1}{x}, y, t, \mu\right)\psi(x, t, \mu), \quad (3.5)$$

where  $\hat{\chi}$  is the “pseudodifferential” operator whose symbol has the following (asymptotic) expansion with respect to the parameter  $\mu$

$$\chi(p, x, y, t, \mu) = \chi_0(p, x, y, t) + \mu\chi_1(p, x, y, t) + \dots. \quad (3.6)$$

From a physical point of view, representation (3.5) means that we “freeze” not only slow variables  $x$  as in formula (3.3), but also slow momenta, which are differential operators  $-i\mu\partial/\partial x$  in quantum mechanics. Note that in many situations the leading term  $\chi_0(p, x, y, t)$  in expansion (3.6) does not depend on  $p$ , but the corrections usually do. This dependence plays an important role when estimating the limits of the adiabatic approximation in concrete problems.

We still do not fix the equation for the function  $\psi$  describing the longitudinal motion. Following the idea of the so-called *Peierls substitution* in solid-state physics (see, *e.g.*, [2, 5, 22]), we assume that the wave function  $\psi$  is a solution of the following equation (describing the longitudinal dynamics):

$$i\mu\psi_t = \hat{L}\psi, \quad \hat{L} = L\left(-i\mu\frac{\partial}{\partial x}, \overset{1}{x}, t, \mu\right), \quad (3.7)$$



where  $\hat{L}$  is a pseudodifferential (sometimes, differential) operator with symbol  $L(p, x, t, \mu)$  having the expansion

$$L(p, x, t, \mu) = L_0(p, x, t) + \mu L_1(p, x, t) + \dots \quad (3.8)$$

The operator  $\hat{L}$  is called the (full) quantum effective Hamiltonian with the principal part  $\hat{L}_0$ . Sometimes, the symbol  $L_0$  is also called an effective classical Hamiltonian and is denoted by  $L_0 = H_{\text{eff}}(p, x, t)$ . The operator  $\hat{\chi}$  will be called an *intertwining* operator (*cf.* [14, 17, 18]). Equation (3.7) can also be understood as the *quantization of the Hamilton–Jacobi equation or the dispersion relation*. The wave function  $\psi$  has different names in different fields. For instance,  $\psi$  is a nuclear function in molecular physics, a longitudinal wave function in waveguides, an electron function in crystals, etc. We shall call it a *wave function of adiabatic motion* and we shall call Equation (3.7) the effective equation of adiabatic motion.

Representation (3.5) together with Equation (3.7) (a generalization of the Peierls substitution) is a formalization of the operator separation of variables in the adiabatic approximation. Of course, the corrections  $L_1, L_2, \dots$  appear in the problems in which the variables cannot be separated exactly.

The reduced Equation (3.7) contains fewer independent variables and hence should be simpler than the original one. Thus, we see (and we mentioned this in the Introduction) that solving the original equation can be divided into two parts: (1) *the “operator (adiabatic) separation of variables” based on formula (3.5), which reduces the original equation to Equation (3.7), and (2) the process of solving this simpler equation.*

The realization of the first step consists in finding the symbols (functions)  $\chi_j$  and  $L_j$ . We shall state the general scheme of their construction and discuss different related questions (*e.g.*, concerning the reasonable number of terms in expansions (3.6), (3.8)) in the next sections. Now we discuss a natural generalization of the operators  $\hat{\chi}$  and  $\hat{L}$ .

It is easy to see that, in the case of exact separation of variables,  $\chi = \chi_0$  is an eigenfunction of some additional spectral problem. The same fact holds for the functions  $\chi_0(x, p, y, t)$ ; later we shall numerate them by a multi-index  $\nu$ . Thus formula (3.5) describes only some special solutions of the original equation corresponding to the term with the index  $\nu$ . It is possible to construct more general ones summing solutions (3.5) with different indices  $\nu$  and the corresponding  $\hat{\chi}, \psi$ . Another conclusion is that, in the case of exact separation of variables, the spectrum of the above-mentioned additional spectral problem can be degenerate and several eigenfunctions can correspond to the same eigenvalue. Then, instead of the product  $\chi(y, \mu)\psi(x, t, \mu)$ , one should write the sum  $\sum_{j=1}^k \chi_j(y, \mu)\psi_j(x, t, \mu)$ , where  $k$  is the multiplicity of the corresponding eigenvalue. The same generalization should be performed in formula (3.5). Also, if the original problem is a vector one (*i.e.*, if (2.2) is a system of PDEs for  $s$  unknown functions), then  $\hat{\chi}_j$  has  $s$  components. Finally, in formula (3.5) and in Equation (3.7) we mean the following:

- (1)  $\hat{\chi}$  is a matrix pseudodifferential operator with  $s$  rows and  $r$  columns,
- (2)  $\psi$  is an  $k$ -dimensional vector function  $\psi = (\psi_1, \dots, \psi_k)^T$ ,
- (3)  $L$  is an  $k \times k$  matrix pseudodifferential operator with the principal symbol  $L_0 = H_{\text{eff}}(p, x)E_k$ , where the number  $r$  determines the multiplicity of the corresponding effective Hamiltonian  $H_{\text{eff}}$  and  $E_k$  is the  $k \times k$  identity matrix. The corrections  $L_j$  usually are not diagonal, which means that interaction is present inside the mode (or the term) determined by this effective Hamiltonian  $H_{\text{eff}}(p, x)$ .

The number of terms in the expansions of the intertwining operator  $\hat{\chi}$  and the operator  $\hat{L}$  (with fixed index  $\nu$ ) can be arbitrarily large. However, it is, as a rule, a very complicated problem to calculate the terms of these series explicitly, even the lower-order terms. Therefore, it

is natural to consider only the terms required to estimate correctly the *leading* term of the asymptotics of the wave function or of the energy value.

However, the notion of the “leading” term of an asymptotics expression can be determined not only by the adiabatic parameter  $\mu$ , but also by the other ones, for instance, by the so-called “semiclassical parameter”  $h$ , which is related to the form of the effective potential and the solution of the reduced Equation (3.7). The appearance of this new parameter is very important for future asymptotic constructions. We shall discuss the corresponding questions in detail later in Section 5. Now we only say that, usually, for the construction of the leading term of an asymptotic solution, it is sufficient to find  $L_0$ ,  $L_1$ , and  $L_2|_{p=0}$ . Another interesting fact is that the effects of a semiclassical splitting of the effective Hamiltonian and a change in the classical characteristics occur in the degenerate case (see Section 4.6).

### 3.3. SCHEME OF THE OPERATOR SEPARATION OF VARIABLES

To simplify the analysis, let us assume that, in Equations (2.2) and (3.1),  $\mathcal{H}$  and the operator  $\hat{\mathcal{H}}$  are essentially self-adjoint. We shall seek the solution of (2.2) in the following form:

$$\Psi_i(x, y, t, \mu) = \sum_{j=1}^k \chi_{ij}(\hat{x}, -i\mu \frac{\partial}{\partial x}, y, t, \mu) \psi_j(x, t, \mu) = (\hat{\chi} \psi)_i, \tag{3.9}$$

where  $\psi = (\psi_1, \dots, \psi_k)^T$  is the wave function of some chosen *term* (or a chosen “fast” mode) with a degeneration multiplicity equal to  $k$  and  $\hat{\chi}$  is an *intertwining* matrix pseudodifferential operator:

$$\hat{\chi} = \begin{pmatrix} \hat{\chi}_{11} & \dots & \hat{\chi}_{1k} \\ \dots & \dots & \dots \\ \hat{\chi}_{s1} & \dots & \hat{\chi}_{sk} \end{pmatrix}, \quad \chi(p, x, y, t, \mu) = \chi_0(p, x, y, t) + \mu \chi_1(p, x, y, t) + \dots \tag{3.10}$$

We assume that the vector function  $\psi$  satisfies the “effective equation of adiabatic motion” (3.7) generated by the matrix operator  $\hat{L}$

$$\hat{L} = \begin{pmatrix} \hat{L}_{11} & \dots & \hat{L}_{1k} \\ \dots & \dots & \dots \\ \hat{L}_{k1} & \dots & \hat{L}_{kk} \end{pmatrix}, \quad L(p, x, t, \mu) = L_0(p, x, t) + \mu L_1(p, x, t) + \dots,$$

where the matrix  $L_0(p, x, t)$  is proportional to the unitary  $k \times k$  matrix  $E_k$ :  $L_0(p, x, t) = H_{\text{eff}} E_k$ . The coefficient of proportionality  $H_{\text{eff}}$  is an *effective Hamiltonian*. Hence the problem is reduced to finding the operators  $\hat{\chi}$  and  $\hat{L}$  or their *symbols*  $\chi$  and  $L$ . Once we have found these, we can reduce the initial problem to a simpler (reduced) Equation (3.7) for the vector function  $\psi$ . The original solution  $\Psi$  can be reconstructed in accordance with (3.9).

Substituting the function  $\Psi$  from (3.9) in (2.2), we obtain:

$$i\mu \hat{\chi} \psi_t + i\mu \hat{\chi}_t \psi = \hat{\mathcal{H}} \hat{\chi} \psi.$$

Using condition (3.7), rewrite this equation in the following form:  $(\hat{\chi} \hat{L} + i\mu \hat{\chi}_t - \hat{\mathcal{H}} \hat{\chi}) \psi = 0$ . A sufficient condition for the last equality to be valid is the operator relation  $\hat{\chi} \hat{L} + i\mu \hat{\chi}_t - \hat{\mathcal{H}} \hat{\chi} = 0$ . Let us pass from operators to symbols [6] in this relation using formula (2.10). This leads to

the equation

$$\begin{aligned} & \chi(p - i\mu \frac{\partial}{\partial x}, \overset{1}{x}, \overset{2}{y}, t, \mu)L(x, p, t, \mu) + i\mu \chi_t(p, x, y, t, \mu) - \\ & - \mathcal{H}(p - i\mu \frac{\partial}{\partial x}, \overset{1}{x}, \overset{2}{y}, t, \mu)\chi(p, x, y, t, \mu) = 0. \end{aligned} \quad (3.11)$$

It can be solved using regular perturbation theory, *i.e.*, expanding the items into series with respect to  $\mu$ . Collecting terms of order  $\mu^0 = 1$ , we obtain a family of spectral problems for the self-adjoint operator  $\mathcal{H}_0(p, x, y, -i\partial/\partial y, t)$  depending on  $x, p, t$ :

$$\mathcal{H}_0(p, x, -i\frac{\partial}{\partial y}, y, t)\chi_0(p, x, y, t) = \chi_0(p, x, y, t)L_0(p, x, t). \quad (3.12)$$

We shall assume that the asymptotics (3.9) is completely determined by the eigenvalue (term)  $H_{\text{eff}}(p, x, t)$  whose multiplicity  $k$  does not depend on  $p, x, t$ . Moreover, we shall assume that the value  $H_{\text{eff}}$  is separated from the other eigenvalues or a part of the spectrum of  $\mathcal{H}_0$  (if the spectrum contains a continuous component) uniformly with respect to  $(p, x, t)$  in a certain fixed domain  $(p, x, t) \in \mathcal{M}$ .

So

$$L_0(p, x, t) = H_{\text{eff}}(p, x, t)E, \quad (3.13)$$

where  $E$  is a unitary  $k \times k$  matrix. The matrix  $\chi_0(x, p, y, t)$  consisting of orthonormal vector columns, *i.e.*, eigenfunctions of the operator  $\mathcal{H}_0$  corresponding to the eigenvalue  $H_{\text{eff}}(x, p, t)$ , is the *intertwining operator* on the proper subspace induced by this eigenvalue. It is natural to assume that  $\chi_0(x, p, y, t)$  depends smoothly on all its arguments.

Collecting terms of order  $\mu$ , we obtain inhomogeneous equations for  $\chi_j$  and  $L_j$ :

$$(\mathcal{H}_0 - H_{\text{eff}}E)\chi_j = F_j - \mathcal{H}_j\chi_0 + \chi_0L_j, \quad j = 1, 2, \dots \quad (3.14)$$

where  $F_j$  depend on  $\chi_0, \dots, \chi_{j-1}$  and  $L_0, \dots, L_{j-1}$ , in particular,

$$\begin{aligned} F_1 = \hat{D}\chi_0, \quad F_2 = \hat{D}\chi_1^\nu - \mathcal{H}_1\chi_1^\nu + \chi_1^\nu L_1 + i \sum_j \left[ \frac{\partial \mathcal{H}_1}{\partial p_j} \frac{\partial \chi_0^\nu}{\partial x^j} - \frac{\partial \chi_0^\nu}{\partial p_j} \frac{\partial L_1}{\partial x^j} \right] \\ + \frac{1}{2} \sum_{i,j} \left[ \frac{\partial^2 \mathcal{H}_0}{\partial p_i \partial p_j} \frac{\partial^2 \chi_0^\nu}{\partial x^i \partial x^j} - \frac{\partial^2 H_{\text{eff}}}{\partial x^i \partial x^j} \frac{\partial^2 \chi_0^\nu}{\partial p_i \partial p_j} \right]. \end{aligned} \quad (3.15)$$

Here

$$\begin{aligned} \hat{D} = i \frac{\partial}{\partial t} + i \sum_j \left[ \frac{\partial \mathcal{H}_0}{\partial p_j} \frac{\partial}{\partial x^j} - \frac{\partial H_{\text{eff}}}{\partial x^j} \frac{\partial}{\partial p_j} \right] = i \frac{d}{dt} + i \sum_j \left[ \frac{\partial \mathcal{H}_0}{\partial p_j} - \frac{\partial H_{\text{eff}}}{\partial p_j} \right] \frac{\partial}{\partial x^j}, \\ \frac{d}{dt} = \frac{\partial}{\partial t} - \sum_j \frac{\partial H_{\text{eff}}}{\partial x^j} \frac{\partial}{\partial p_j} + \sum_j \frac{\partial H_{\text{eff}}}{\partial p_j} \frac{\partial}{\partial x^j}. \end{aligned}$$

Due to the self-adjointness of the operator  $(\mathcal{H}_0 - H_{\text{eff}}E)$  and the Fredholm alternative, the solvability condition for this equation is equivalent to the condition that its right-hand part is orthogonal to the vector-columns of the matrix  $\chi_0$ . It follows that  $L_j = \langle \chi_0^T, \mathcal{H}_j \chi_0 \rangle|_y - \langle \chi_0^T, F_j \rangle|_y$ . In particular, one can obtain:

$$L_1 = \left\langle \chi_0^T, \mathcal{H}_1 \chi_0 \right\rangle_y - i \left\langle \chi_0^T, \frac{d\chi_0}{dt} \right\rangle_y - i \left\langle \chi_0^T, \sum_{j=1}^n \left[ \frac{\partial \mathcal{H}_0}{\partial p_j} - \frac{\partial H_{\text{eff}}}{\partial p_j} \right] \frac{\partial \chi_0}{\partial x^j} \right\rangle_y. \quad (3.16)$$

Assuming that  $L_1$  has form (3.16), one can find the correction, *i.e.*, the matrix  $\chi_1 = (\mathcal{H}_0 - H_{\text{eff}}E)^{-1}(F_1 - \mathcal{H}_1\chi_0 + \chi_0L_1)$ , fixing it for determinacy by means of the condition of orthogonality of vector-columns of the matrices  $\chi_0$  and  $\chi_1$ . Repeating this procedure leads to calculation of  $L_j, \chi_j$ . Formulas (3.13), (3.16), etc. give the expansion coefficients of the symbol of the reduced Equation (3.7). Note that the construction of the correction  $L_1$  includes only functions of zero approximation (like in standard perturbation theory). In general, the symbol  $L_2$  includes  $\chi_1$ , so, to find it, one has to invert the operator  $(\mathcal{H}_0 - H_{\text{eff}}E)$ .

### 3.3.1. Remark 1

The methods from [14] allow one to consider more general situations in which the quantum Hamiltonian  $\hat{\mathcal{H}}(\hat{p}, \hat{x}, \hat{p}_y, \hat{y}, \mu)$  is a function of vector operators  $(\hat{p}, \hat{x}, \hat{p}_y, \hat{y})$  with commutator relations  $[\hat{x}_j, \hat{p}_j] = i\mu$ ,  $[\hat{y}_j, \hat{p}_{yj}] = i$ ,  $\mu \ll 1$ , or even more complicated ones (see Example in Section 4.2). However, in this paper we basically consider the situation in which  $\hat{x} = x$ ,  $\hat{p}_x = -i\mu\partial/\partial x$ .

### 3.3.2. Remark 2

It is not difficult to modify the presented formal scheme for the non-self-adjoint original operator  $\mathcal{H}$ . In particular, one has to use the eigenfunctions of the adjoint operator in the orthogonality conditions. But, of course, it is necessary to add some additional conditions like the existence of real-valued effective Hamiltonians, etc. (see Example in Section 4.3).

### 3.3.3. Remark 3 Operator separation of variables and adiabatic approximation in classical mechanics

There exist a certain classical analog of the adiabatic approach based on the ‘‘operator separation of variables’’ ([23–27]). The main idea can be illustrated by means of the Hamiltonian  $\mathcal{H}(\mu p_x, x, p_y, y, \mu)$  with a small parameter  $\mu$ . If we change the variables  $x, p_x$  by  $\xi = x/\mu$  and  $p_\xi = \mu p_x$ , then we obtain a Hamiltonian of the form  $\mathcal{H}(p, \mu\xi, p_y, y, \mu)$ . It is convenient to write the Hamiltonian in noncanonical variables  $x$  and  $p$ ,  $dp \wedge dx = \mu dp_x \wedge dx = \mu dp \wedge d\xi$ :  $\mathcal{H}(p, x, p_y, y, \mu)$ . The Hamiltonian equations for the variables  $p, x, p_y, y$  have the form

$$\dot{x} = \mu \frac{\partial \mathcal{H}}{\partial p_\xi} \ll 1, \quad \dot{p} = -\mu \frac{\partial \mathcal{H}}{\partial x} \ll 1, \quad \dot{y} = \frac{\partial \mathcal{H}}{\partial p_y}, \quad \dot{p}_y = -\frac{\partial \mathcal{H}}{\partial y}. \quad (3.17)$$

Since we have  $\dot{p}, \dot{x} \sim \mu$  for the derivatives, while  $\dot{p}_y, \dot{y} \sim 1$ , it is natural to say that the variables  $p, x$  are ‘‘slow variables’’ and the variables  $p_y, y$  are ‘‘fast variables.’’ Taking into account that there are variables of two types, it is natural to ‘‘freeze’’ slow variables and obtain a family of Hamiltonians with  $k$  degrees of freedom depending on the parameters  $(p, x)$ . We do not consider resonance problems and restrict our consideration to the case in which  $k = 1$  and  $(p_y, y) \in \mathbb{R}^2$ . Let us assume that, in some domain  $(p, x) \in \Omega$ , the trajectories of  $\mathcal{H}(\{p, x\}, p_y, y, 0)$  are closed. The braces  $\{\cdot\}$  mean that the included variables are considered as parameters (*i.e.*, are ‘‘frozen’’). Then it is possible to introduce ‘‘action-angle’’ variables  $(J, \varphi)$  corresponding to these closed trajectories. The passage to these variables is determined by the change of variables  $y = Y_0(J, \varphi, p, x)$ ,  $p_y = P_y^0(J, \varphi, p, x)$ . Unfortunately, this change of variables is not canonical and, to make it canonical, one has to add corrections and write  $y = Y_0(J, \varphi, P, X) + \mu Y_1(J, \varphi, P, X) + \dots$ ,  $p_y = P_y^0(J, \varphi, P, X) + \mu P_y^1(J, \varphi, P, X) + \dots$ ,  $p = P + \mu P_1(J, \varphi, P, X) + \dots$ , and  $x = X + \mu X_1(J, \varphi, P, X) + \dots$ . Then the original Hamiltonian can be written in the form

$$\begin{aligned}
 \mathcal{H}(J, \varphi, P, X) &= \mathcal{H}_0(J, P, X) + \mu \left[ \frac{\partial \mathcal{H}_0}{\partial y}(P, X, P_y^0, Y_0) Y_1 + \frac{\partial \mathcal{H}_0}{\partial p_y}(P, X, P_y^0, Y_0) P_y^1 \right. \\
 &\quad \left. + \frac{\partial \mathcal{H}_0}{\partial x}(P, X, P_y^0, Y_0) X_1 + \frac{\partial \mathcal{H}_0}{\partial p}(P, X, P_y^0, Y_0) P^1 + \mathcal{H}_1(P, X, P_y^0, Y_0) \right] + O(\mu^2), \\
 P_y^1 &= P_y^1(J, \varphi, P, X), \quad Y_1 = Y_1(J, \varphi, P, X), \quad P^1 = P^1(J, \varphi, P, X), \quad X_1 = X_1(J, \varphi, P, X) \\
 P_y^0 &= P_y^0(J, \varphi, P, X), \quad Y_0 = Y_0(J, \varphi, P, X),
 \end{aligned} \tag{3.18}$$

where  $\mathcal{H}(p, x, p_y, y, \mu) = \mathcal{H}_0(p, x, p_y, y) + \mu \mathcal{H}_1(p, x, p_y, y) + O(\mu^2)$ . Now we have a typical problem from averaging theory. After averaging, we obtain two terms of the expansion of the effective Hamiltonian  $L(J, P, X, \mu) = L_0(J, P, X) + \mu L_1(J, P, X) + O(\mu^2)$ :

$$\begin{aligned}
 L_0(J, P, X) &= \mathcal{H}_0(J, P, X), \\
 L_1(J, P, X) &= \int_0^{2\pi} d\varphi \left[ \frac{\partial \mathcal{H}_0}{\partial y}(P, X, P_y^0, Y_0) Y_1 + \frac{\partial \mathcal{H}_0}{\partial p_y}(P, X, P_y^0, Y_0) P_y^1 \right. \\
 &\quad \left. + \frac{\partial \mathcal{H}_0}{\partial x}(P, X, P_y^0, Y_0) X_1 + \frac{\partial \mathcal{H}_0}{\partial p}(P, X, P_y^0, Y_0) P^1 + \mathcal{H}_1(P, X, P_y^0, Y_0) \right], \tag{3.19}
 \end{aligned}$$

so  $J = \text{const}$  and the integration of the original system is reduced to solving a system with  $n$  degrees of freedom. The action  $J$  corresponds to the “quantum” number  $\nu$  of the term  $\chi^\nu$ , the term  $\int_0^{2\pi} d\varphi \mathcal{H}_1(P, X, P_y^0(J, \varphi, P, X), Y_0(J, \varphi, P, X))$  corresponds to  $\langle \chi_0, \mathcal{H}_1 \chi_0 \rangle_y$ , and the corrections related to the canonical change of variables in the classical problem correspond to other terms in  $L_1$  in quantum problem. Of course, this is simply an analogy (*cf.* [7, 28, 29], etc.).

### 3.3.4. Remark 4

The classical analogue of the reduction at the first stage is well known [37]: excluding the fast variables, we obtain a system in the zeroth approximation with holonomic constraints; this system is equivalent to the  $n$ -dimensional Lagrangian system. Thus, the adiabatic reduction to (3.7) could be interpreted as the “excluding of quantum constraints” (see [30–36]). But the classical system corresponding to the reduced quantum system generally does not coincide with the result of the classical reduction (in the sense [37]). Moreover, the classical systems arising in the adiabatic reduction turn out to be different for different relations between  $\mu$  and “semiclassical” parameter  $\hbar$ , which will be introduced in Section 5; using the terminology of [15, 38], we can say that they correspond to different nonstandard characteristics of the quantum problem. For example, the classical equation of motion in nanotubes can sometimes include terms arising because spin exists. This is explainable physically because longitudinal motion is already determined by rather small energies that are quite comparable to the spin energy.

### 3.3.5. Remark 5

In some problems one can apply the semiclassical approximation to solve (3.12) (see *e.g.* [13, 39]).

## 4. Examples of problems with operator-valued symbols and parameters

Let us illustrate the general scheme with several examples.

## 4.1. EQUATION WITH RAPIDLY OSCILLATING COEFFICIENTS AND ELECTRON WAVES IN CRYSTALS

One encounters equations with rapidly oscillating coefficients in many problems of solid physics and continuum mechanics. For instance, these types of equations describe propagation of electron waves in crystals, of elastic waves in composite materials, etc. For constructing asymptotic solutions to equations with rapidly oscillating coefficients, there exist different approaches depending on their behavior and properties. Among these approaches, one can at least mention averaging methods, homogenization, and adiabatic approximation. There exists a very extensive literature concerning this topic and a review of all these approaches will not be attempted here. We only want to show that one can look at equations with rapidly oscillating coefficients as equations with operator-valued symbols [11, 12] and, for the construction of their asymptotics, use the method described in Section 4. Here we refer only to the general monographs [1, 3, 40–42] and closely related papers [43–45].

As an example, we consider the Schrödinger equation with a fast oscillating potential

$$i\mu\psi_t = -\frac{\mu^2}{2}\Delta\psi + v\left(\frac{\Phi(x)}{\mu}, x\right), \quad x \in \mathbb{R}^n, \quad \Phi \in \mathbb{R}^m, \quad (4.1)$$

where  $v(y, x)$  is a smooth function that is  $2\pi$ -periodic with respect to each “fast” variable  $y_j$ ,  $j=1, \dots, m$ . The given phases  $\Phi_j(x)$  are smooth functions. Generally speaking, their number  $k$  can be arbitrary. In some problems, the phases are linear functions  $\Phi_j = \langle k_j, x_j \rangle$ ; the nonlinear phases  $\Phi_j$  describe the case of a nonuniform potential  $v$ . The additional dependence of the potential on the variable  $x$  implies its slow deformation. Equation (4.1) with such a potential simulates the propagation of electron waves in a lattice or, for instance, if  $m=1$ , in stratified media. The simplest example of a rapidly oscillating potential is given by the formula ( $n=1, m=1$ ):  $v = v_0(x) + a(x) \cos \frac{\Phi(x)}{\mu}$ , where  $v_0(x), a(x)$  are smooth functions.

Let us find the unknown function  $\psi(x, t, \mu)$  in the form

$$\psi(x, t, \mu) = \Psi\left(\frac{\Phi(x)}{\mu}, x, t, \mu\right), \quad (4.2)$$

where the new unknown function  $\Psi(y, x, t, \mu)$  is  $2\pi$ -periodic with respect to each variable  $y_j$ . Substituting (4.2) in (4.1), we see that the function  $\psi(x, t, \mu)$  (4.2) satisfies (4.1) if the function  $\Psi(y, x, t, \mu)$  is a solution of (2.2) with

$$\hat{\mathcal{H}} = \left(-i\mu \frac{\partial}{\partial x} - i \frac{\partial \Phi}{\partial x} \frac{\partial}{\partial y}\right)^2 + v(y, x). \quad (4.3)$$

We again see that the small parameter  $\mu$  is located in front of the derivative  $\partial/\partial x$ , but there is no small parameter in front of the derivative  $\partial/\partial y$ . Thus the equation with Hamiltonian (4.3) is an equation with an operator-valued symbol, namely,

$$\mathcal{H} = \mathcal{H}_0 - \mu \sum_{j=1}^m \Delta \Phi_j \frac{\partial}{\partial y_j}, \quad \mathcal{H}_0 = \left(p - i \sum_{j=1}^m \frac{\partial \Phi_j}{\partial x} \frac{\partial}{\partial y_j}\right)^2 + v(y, x). \quad (4.4)$$

For each fixed  $(p, x)$ , the operator  $\mathcal{H}$  acts in the  $L_2$ -space on a  $k$ -dimensional torus.

If the vectors  $\partial \Phi_j / \partial x$  are linearly independent for each  $x$ , then the spectrum of the operator  $\mathcal{H}$  is discrete, but, to obtain the reduced equation, one must also use the assumption that the multiplicity of eigenvalues is independent of  $(p, x)$ . In particular, if  $m=1$  and  $\partial \Phi / \partial x \neq 0$ , the spectral problem (3.12) for determining the effective Hamiltonians is a periodic problem and can be reduced to the 1-D Schrödinger equation on a circle for Bloch solutions (see [21,

46]). To realize this reduction, we change the variables in the equation  $\mathcal{H}_0\chi_0 = H_{\text{eff}}\chi_0$  for  $\chi_0$  and  $H_{\text{eff}}$  as follows:

$$y = U\xi, \quad \chi_0 = ue^{-iP\xi}, \quad U = \left| \frac{\partial\Phi}{\partial x} \right|,$$

and put

$$P = P(p, x) \equiv \left\langle \frac{\partial\Phi_j}{\partial x}, p \right\rangle \left/ \left| \frac{\partial\Phi}{\partial x} \right|^2 \right. . \quad (4.5)$$

Then this equation takes the form

$$-u_{\xi\xi} + v(U\xi, x)u = \mathcal{E}u, \quad \mathcal{E} = H_{\text{eff}} - p^2 + P^2,$$

and the periodicity condition becomes the Bloch condition:

$$u(\xi + 2\pi/U, x) = e^{2\pi iP}u(\xi, x).$$

The variable  $x$  is contained in the reduced problem as a parameter. The variable (number)  $P$  is called the *quasi-momentum* of the corresponding Bloch solution. It is a well-known fact that the spectrum of the operator  $-\partial^2/\partial\xi^2 + v(U\xi, x)$  on a circle consists of bands and gaps. Let us enumerate the bands by the number  $\nu$  and denote the ends of the  $\nu$ th band by  $E_-^\nu$  and  $E_+^\nu$ . The spectral parameter  $\mathcal{E}$  and the quasi-momentum  $P$  in each  $\nu$ th band are connected by the *dispersion relation*

$$\mathcal{E} = \mathcal{E}^\nu(P, x).$$

The assumption on the potential  $v(y, x)$  that the  $\nu$ th effective Hamiltonian (eigenvalue) of the operator  $\mathcal{H}^\nu$  is simple (or does not intersect with other effective Hamiltonians at some points  $(p, x)$ ) is equivalent to the assumption that, for each  $x$ , the  $\nu$ th band *does not stick together with the  $\nu - 1$ st and  $\nu + 1$ st bands*. Under this assumption, one can find the reduced equation describing solutions corresponding to the  $\nu$ th term (effective Hamiltonian)

$$H_{\text{eff}}^\nu = \mathcal{E}^\nu(P(p, x), x) + p^2 - (P(p, x))^2.$$

The corresponding function  $\chi_0^\nu(y, p, x)$  is expressed via the Bloch function  $u^\nu$ ,  $u^\nu(\xi, P, x)$ , by the formula

$$\chi_0 = u^\nu \left( \frac{y}{U}, P(p, x), x \right) \exp \left( -i \frac{P(p, x)y}{U} \right).$$

If  $n = 1$  and  $\Phi = x$ , then  $P = p$ , which leads to the following well-known fact in solid state physics: the quasi-momentum becomes the momentum for the equation for electron waves in crystals. In contrast to Examples 1, 2, and 3, the effective Hamiltonian here is not a polynomial in  $p$  and the function  $\chi_0$  depends on the momentum  $p$ .

Let us write the first correction  $L_1$  to the effective Hamiltonian. Using formula (3.16) we obtain

$$L_1 = \left\langle \chi_0, \frac{d\chi_0}{dt} \right\rangle + \left\langle \chi_0, \left( 2p - \frac{\partial H}{\partial p} \right) \nabla \chi_0 \right\rangle + 2i\Re \left\langle \nabla \chi_0 \frac{\partial \chi_0}{\partial y}, \nabla \chi_0 \right\rangle.$$

Note that it is possible to meet a situation in which the number of phases in the potential is greater than the dimension of the configuration space  $n$ . For instance, consider the case  $m = 2$ ,  $n = 1$ . In this situation, the operator  $\mathcal{H}$  is degenerate and its spectrum has a rather

complicated structure. In particular, the spectrum can be a set that is dense everywhere on the spectral axis (the so-called devil's stair) and the multiplicity of its eigenvalues can depend on  $x$ . These problems are related to different types of complicated resonances and to problems with intersecting characteristics. Some results for the solutions of the Cauchy problem in this situation are obtained in [12, 21, 46].

*Remark: Bloch electrons in a weak magnetic field and the Peierls substitution*

The original Peierls substitution was first proposed for the problem with Bloch electrons in a weak magnetic field (see, e.g., [5]). Using the terminology of this paper, this problem can be stated as a spectral problem for the magnetic Schrödinger operator with the periodic electric potential:

$$\hat{\mathcal{H}} = \frac{1}{2} \left( -i\mu \frac{\partial}{\partial x} - A(x) \right)^2 + v \left( \frac{x}{\mu} \right), \quad \langle \nabla, A \rangle = 0.$$

For simplicity, we restrict ourselves to a simple cubic lattice, *i.e.*, assume that  $v = v(y_1, y_2, y_3)$  is  $2\pi$ -periodic with respect to each variable  $y_j = x_j/\mu$ ,  $j = 1, 2, 3$ . The fact that the magnetic field is weak means that  $A(x)$  does not contain any irregular dependence on the parameter  $\mu$  in contrast to the crystalline potential  $v(x/\mu)$ . After the space regularization (4.2) with phase vector  $\Phi(x) \equiv x$  similarly to (4.3), we obtain the problem with operator-valued symbol  $\mathcal{H} = (1/2)(p - i\partial/\partial y - A)^2 + v(y)$ . The procedure based on the formulas (4.5) leads to the problem for Bloch solutions for the operator  $\mathcal{H} = -(1/2)\Delta_y + v(y)$ . Let  $\mathcal{E} = \mathcal{E}^v(P)$ ,  $P = (P_1, P_2, P_3)$  determine the dispersion relation for the Bloch solutions with quasi-momentum  $P$ . Then, according to this subsection,  $L_0^v \equiv H_{\text{eff}}^v = \mathcal{E}^v(p - A)$ ,  $L_1^v = [\text{tr}(\frac{\partial^2 \mathcal{E}^v}{\partial p^2} \frac{\partial A}{\partial x})](p - A)$ , and in (3.7)  $\hat{L} = \hat{L}_0^v + \mu \hat{L}_1^v + O(\mu^2) = \mathcal{E}^v(-i\mu \frac{\partial}{\partial x} - A) + O(\mu^2)$  which is exactly the *Peierls substitution*. The higher order corrections look much more complicated than the leading term [47]. It seems to us that our approach allows one to calculate these corrections more easily than in [47]. Semiclassical analysis of the reduced Equation (3.7) reveals a very complicated and striking topology of surfaces that are invariant to the corresponding phase flow. Recent results and a bibliography can be found in [48].

#### 4.2. ELECTRON-PHONON INTERACTION

As was noted in Remark 1 in Section 3.3.3, one can consider adiabatic problems as problems containing “slightly noncommuting” operators. In the zeroth-order approximation, these operators can be substituted by “ $c$ -numbers,” which allows one to determine a term. For “slightly noncommuting” operators, there are physical quantities that are slowly varying in time. The slightly commuting operators can generate a certain Lie algebra. In the simplest case, this Lie algebra is the Heisenberg algebra, and we can directly use the scheme and formulas proposed in Section 3. Sometimes, it is possible to consider the same problem from a different angle, which depends on the choice of the operators. For instance, to simplify the form of the original Hamiltonian, one can use a (noncanonical) change of variables, which, in turn, leads to the replacement of the Heisenberg commutation relations by different ones. We consider such an example which can be analyzed from these different viewpoints, but since the study of problems based on non-Heisenberg commutation relations requires new nontrivial algebraic and geometric constructions, we restrict ourselves to the approach described in Section 3, although, from some viewpoint, the approach based on non-Heisenberg commutation relations can be more readily realized in some concrete problems.

The electron-phonon interaction is the interaction between light fermions (electrons) and heavy bosons (phonons). Here the lattice modes (bosons) are slow and the electrons



(fermions) are fast. The Hamiltonian of electron-phonon interaction is (see, e.g., [49])

$$\hat{\mathcal{H}} = \sum_n \hat{c}_n (\hat{\psi}_{n+1}^+ \hat{\psi}_n + \hat{\psi}_n^+ \hat{\psi}_{n+1}) + \sum_n K (\hat{x}_{n+1} - \hat{x}_n)^2 + \hat{p}_n^2/2, \quad (4.6)$$

$$[\hat{x}_n, \hat{p}_{n'}] = i\mu\delta_{nn'}, \quad \mu = \hbar/\alpha\sqrt{m_0c_0}, \quad (4.7)$$

$$[\hat{\psi}_j^+, \hat{\psi}_k]_+ \equiv \hat{\psi}_j^+ \hat{\psi}_k + \hat{\psi}_k^+ \hat{\psi}_j = i\delta_{jk}.$$

Here  $m_0, c_0, K, \alpha$  are physical constants; moreover,  $\mu \ll 1$ ; the linear operators  $\hat{\Psi}_1^+, \dots, \hat{\Psi}_M^+$  and  $\hat{\Psi}_1, \dots, \hat{\Psi}_M$  act on the Hilbert space  $\mathbb{H}_1$ , the linear operators  $\hat{p}_1, \dots, \hat{p}_M$  and  $\hat{x}_1, \dots, \hat{x}_M$  act on the Hilbert space  $\mathbb{H}_2$ . The full quantum Hamiltonian  $\hat{\mathcal{H}}$  acts on the Hilbert space  $\mathbb{H} = \mathbb{H}_1 \otimes \mathbb{H}_2$ . The typical situation is given by the operators

$$\hat{c}_n = f(\hat{x}_{n+1} - \hat{x}_n), \quad (4.8)$$

where  $f(z)$  is a smooth function; in particular,  $\hat{c}_n = 1 - \alpha(\hat{x}_{n+1} - \hat{x}_n)$ . Let us set  $\hat{X} = (\hat{x}_1, \dots, \hat{x}_N)$ ,  $\hat{P} = (\hat{p}_1, \dots, \hat{p}_N)$ ,  $\hat{\Psi} = (\hat{\psi}_1, \dots, \hat{\psi}_M)$ ,  $\hat{\Psi}^+ = (\hat{\psi}_1^+, \dots, \hat{\psi}_M^+)$ . In a more general case, the Hamiltonian  $\hat{\mathcal{H}}$  of electron-phonon interaction can be written as

$$\hat{\mathcal{H}} = \langle \hat{\Psi}^+, \mathcal{L}(\hat{X}, \hat{P}) \hat{\Psi} \rangle + \Phi(\hat{X}) + \hat{P}^2/2, \quad (4.9)$$

where  $\mathcal{L}(P, X)$  is a Hermitian  $M \times M$  matrix with coefficients depending on  $X$  and  $P$ , and the operator  $\mathcal{L}(\hat{X}, \hat{P})$  is understood in the sense of Weyl calculus (see [14, 17, 18]). To simplify the consideration, we restrict ourselves to the case in which  $\mathcal{L} = \mathcal{L}_1(X) + \mathcal{L}_2(P)$ ; then the question about the ordering of the operators  $\hat{X}$  and  $\hat{P}$  does not appear. As we have just said, it is possible to develop the ‘‘operator separation of variables’’ based on the algebra of operators  $\hat{c}_j, \hat{p}_j$  with the commutation relations

$$[\hat{p}_j, \hat{c}_k] = i\mu(\delta_{jk} - \delta_{jk+1})\hat{c}_k,$$

but here we use the standard representation  $\hat{x}_j = x_j$  and  $\hat{p}_j = -i\mu\partial/\partial x_j$  and close the lattice by the Born–Kármán periodicity condition identifying the operators with the numbers  $j$  and  $j + M$ .

Denote the electron-phonon wave function by  $\Upsilon$  and consider the stationary problem

$$\hat{\mathcal{H}}\Upsilon = \mathcal{E}\Upsilon, \quad \Upsilon \in \mathbb{H}. \quad (4.10)$$

We have an equation with operator-valued symbol which, obviously, is the operator

$$\mathcal{H}(X, P) = \langle \Psi^+, \mathcal{L}(X, P) \Psi \rangle + (\Phi(X) + P^2/2)\hat{I}_1 \quad (4.11)$$

acting on the Hilbert space  $\mathbb{H}_1$ . We also denote the identity operator acting on  $\mathbb{H}_j$  by  $\hat{I}_j$ .

To realize the scheme of the operator separation of variables, it is necessary to find the spectrum of the operator-valued symbol  $\mathcal{H}(X, P)$ . A nice fact is that this spectrum can be expressed via the eigenvalues of the matrix  $\mathcal{L}$ . Namely, suppose that  $\psi(E_j) = (\psi_1(E_j), \dots, \psi_M(E_j))$  are the eigenvectors of the matrix  $\mathcal{L}(X, P)$  corresponding to its eigenvalues  $E_j(X, P)$   $E_1 \leq \dots \leq E_M$  and satisfying the normalization conditions  $\langle \psi(E_j), \psi(E_k) \rangle = \delta_{jk}$ . Using the basis  $\{\psi(E_j)\}$ , one can expand the operators  $\hat{\Psi}^+$  and  $\hat{\Psi}$

$$\hat{\psi}^+ = \sum_{j=1}^M \psi^*(E_j) \hat{a}_j^+, \quad \hat{\psi} = \sum_{j=1}^M \psi(E_j) \hat{a}_j. \quad (4.12)$$

The coefficients (operators) of this expansion,  $\hat{a}_j^+$  and  $\hat{a}_j$ , are called the creation and annihilation operators [50]. They determine the operators of the number of particles  $\hat{N}_j = \hat{a}_j^+ \hat{a}_j$ . Finally, the operator-valued symbol can be written as

$$\mathcal{H}(X, P) = \sum_{j=1}^M E_j(X, P) \hat{N}_j + \Phi(X) + P^2/2, \quad \hat{N}_j = \hat{a}_j^+ \hat{a}_j.$$

From this, we find the  $\nu$ th effective Hamiltonian

$$H_{\text{eff}}^\nu(X, P) = \sum_{j=1}^{\nu} E_j(X, P) + \Phi(X) + P^2/2, \quad (4.13)$$

and the symbols of the corresponding intertwining operators  $\chi_0^\nu$ :

$$\chi_0^\nu = \hat{N}_1 \dots \hat{N}_\nu (I - \hat{N}_{\nu+1}) \dots (I - \hat{N}_M) \cdot 1. \quad (4.14)$$

Let us analyze the formula for  $L_1$ . If the effective Hamiltonian  $H_{\text{eff}}^\nu$  is degenerate or  $\mathcal{L}_1(X), \mathcal{L}_2(P)$  are complex matrices, one must use the general formula (3.16). For the case in which  $\mathcal{L}_2(P) = 0$  and  $\mathcal{L}_1(X)$  is a real-valued matrix and its spectrum  $(E_1(x), \dots, E_M(x))$  is nondegenerate, it follows from formulas (4.13) that the effective Hamiltonians are nondegenerate and  $H_{\text{eff}}^\nu$  and  $\chi_0^\nu$  are real. Thus, taking into account the relations  $\mathcal{H}_1 = 0$ ,  $\left\langle \chi_0^T, \frac{d\chi_0}{dt} \right\rangle_y = \frac{1}{2} \frac{d}{dt} \langle \chi_0^T, \chi_0 \rangle_y = 0$ ,  $\frac{\partial \mathcal{H}_0}{\partial p_l} - \frac{\partial H_{\text{eff}}}{\partial p_l} I = 0$ , we obtain

$$L_1 = 0.$$

This equality holds for the operators  $\hat{c}_n$  given by formula (4.8), in particular, if  $c_n = e^{x_n - x_{n-1}}$ .

It was pointed out that in this case it is possible to relate problem (4.10) to the integrable Toda lattice model [51, 52]. Then this observation was used to construct its semiclassical asymptotics [53], and at the same time, commutation relations of different type were chosen.

#### 4.3. INTERNAL WAVES IN THE OCEAN IN A PYCNOCLINE

The next example concerns a situation in which the operator  $\mathcal{H}$  is not self-adjoint; moreover, the system of equations under study differs somewhat from (2.2). Thus the scheme of Section 3 requires a slight modification.

We consider a system of hydrodynamic equations for an ideal incompressible liquid linearized on the flow with velocity  $U$  and density  $\rho_0$ . Let  $x = (x_1, x_2)$  be the horizontal coordinates,  $z$  be the vertical coordinate,  $u = (u_1, u_2, u_3)$ , and  $\rho$  perturbations of the velocity and density,  $\Pi$  the pressure and  $g = (0, 0, |g|)$  the gravity acceleration. We introduce dimensionless variables and parameters by the formulas:  $U = U' \omega_1 \lambda$ ,  $u = u' \omega_1 \lambda$ ,  $t = t' \omega_2$ ,  $x = x' L$ ,  $z = z' L$ ,  $g = g' \omega_1^2 \lambda$ ,  $\Pi = \Pi' \omega_1^2 \lambda^2$ , and  $\rho_0 = \rho_0' \bar{\rho}$ ,  $\rho = \rho' \bar{\rho}$ , where  $\omega_1$  is the characteristic frequency of the internal wave,  $\lambda$  is the characteristic wavelength,  $L$  is the characteristic distance in the horizontal direction within which the characteristics of the liquid vary,  $\omega_2$  is the average value of the Väisälä–Brunt frequency,  $\bar{\rho}$  and  $\omega_1^2 \lambda^2$  are the characteristic values of density and pressure, and  $\mu = \lambda/L = \omega_1/\omega_2 \ll 1$  is a small parameter.

In dimensionless variables, the linearized system for waves in liquids has the form [10, 54]:

$$\begin{cases} \mu \rho_0 \frac{\partial u}{\partial t} + \mu \rho_0 \langle U, \nabla \rangle u + \mu \rho_0 \langle u, \nabla \rangle U + \mu \nabla \Pi + \rho g = 0, \\ \mu \frac{\partial \rho}{\partial t} + \mu \langle U, \nabla \rangle \rho + \mu \langle u, \nabla \rangle \rho_0 = 0, \\ \mu \langle \nabla, u \rangle = 0, \end{cases} \quad (4.15)$$

where  $\langle \cdot, \cdot \rangle$  is the inner product in  $\mathbb{R}^3$ . The difference between (4.15) and (2.2) is that the last equation of this system contains the time-derivative.

We shall consider that the width of the pycnocline  $\Delta z \sim \mu$ , and that the depth of its location varies at distances  $\sim 1$ , i.e.,  $\rho_0 = \rho_0(z/\mu - f(x), x)$  (the equation for the surface of a pycnocline is  $z = \mu f$ ). The functions  $U(x) = (U_1, U_2, 0)$ ,  $\rho_0(y, x)$ ,  $f(x)$  are assumed to be smooth,  $0 < \delta_0 < \rho_0 < c_0$  ( $\delta_0$ ,  $c_0$  are constants), the square of the Väisälä–Brunt frequency  $\omega_0^2 = -|g| \frac{\partial \rho_0}{\partial y} / \rho_0$  is positive and vanishes rather fast as  $|y| \rightarrow \infty$ . We assume that the functions  $u_j$  and  $\rho$  decay quite fast as  $|z| \rightarrow \infty$ . The other boundary and initial conditions for (4.15) are chosen in a special way and should be formulated for the corresponding reduced effective equation of adiabatic motion (3.3).

Let us introduce a new independent variable  $y = z/\mu - f(x)$  and a vector with five components  $\Psi(x, y, t, \mu) = (u, \rho, \Pi)$ . We must substitute the differential operators as  $\frac{\partial}{\partial x_i} \rightarrow \frac{\partial}{\partial x_i} - \frac{\partial f}{\partial x_i} \frac{\partial}{\partial y}$  and  $\mu \frac{\partial}{\partial z} \rightarrow \frac{\partial}{\partial y}$  in the equations for the vector  $\Psi$ . Then, for  $\Psi$ , we obtain a system of equations containing “fast” variable  $y$  and slow variables  $x$ ,  $t$ . For convenience, we multiply this system by  $i = \sqrt{-1}$ :

$$i\mu B\Psi_t = \mathcal{H} \left( \frac{\partial}{\partial x}, -i\mu \frac{\partial}{\partial x}, y, -i \frac{\partial}{\partial y}, \mu \right) \Psi(x, y, t, \mu), \quad B = \begin{pmatrix} \rho_0 & 0 & 0 & 0 & 0 \\ 0 & \rho_0 & 0 & 0 & 0 \\ 0 & 0 & \rho_0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}. \quad (4.16)$$

The matrix symbols  $\mathcal{H}_0$  and  $\mathcal{H}_1$  have the form

$$\mathcal{H}_0 \left( x, p, y, -i \frac{\partial}{\partial y}, t \right) = \begin{pmatrix} \rho_0 \langle U, p \rangle & 0 & 0 & 0 & p_1 \\ 0 & \rho_0 \langle U, p \rangle & 0 & 0 & p_2 \\ 0 & 0 & \rho_0 \langle U, p \rangle & -i|g| & -i \frac{\partial}{\partial y} \\ 0 & 0 & -i \frac{\partial \rho_0}{\partial y} & \langle U, p \rangle & 0 \\ p_1 & p_2 & -i \frac{\partial}{\partial y} & 0 & 0 \end{pmatrix},$$

$$\mathcal{H}_1 = -i\rho_0 \begin{pmatrix} \frac{\partial U_1}{\partial x_1} & \frac{\partial U_1}{\partial x_2} & 0 & 0 & 0 \\ \frac{\partial U_2}{\partial x_1} & \frac{\partial U_2}{\partial x_2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 & 0 & \frac{\partial f}{\partial x_1} (i \frac{\partial}{\partial y}) \\ 0 & 0 & 0 & 0 & \frac{\partial f}{\partial x_2} (i \frac{\partial}{\partial y}) \\ 0 & 0 & 0 & 0 & 0 \\ -i \frac{\partial \rho_0}{\partial x_1} + i \frac{\partial f}{\partial x_1} \frac{\partial \rho_0}{\partial y} & -i \frac{\partial \rho_0}{\partial x_2} + i \frac{\partial f}{\partial x_2} \frac{\partial \rho_0}{\partial y} & 0 & 0 & 0 \\ \frac{\partial f}{\partial x_1} (i \frac{\partial}{\partial y}) & \frac{\partial f}{\partial x_2} (i \frac{\partial}{\partial y}) & 0 & 0 & 0 \end{pmatrix} + \langle U, \nabla f \rangle B \left( i \frac{\partial}{\partial y} \right),$$

where  $p = (p_1, p_2, 0)$ . Let us show that the general scheme of the operator separation can be easily modified for this situation, although one of the equations in the system does not contain the time-derivative.

We seek the solution in the form (3.9) and assume that  $\psi(x, t, \mu)$  satisfies an effective equation of the form (3.3). Then, instead of (3.11), we obtain the following relation

$$B\chi \left( \frac{2}{x}, p - i\mu \frac{\partial}{\partial x}, y, t, \mu \right) L(x, p, t, \mu) + i\mu B\chi_t(x, p, t, y, \mu) - \mathcal{H} \left( \frac{2}{x}, p - i\mu \frac{\partial}{\partial x}, y, -i \frac{\partial}{\partial y}, t, \mu \right) \chi(x, p, y, t, \mu) = 0.$$

Expanding this relation into a series with respect to a small parameter  $\mu$ , instead of the eigenvalue problem, we obtain the problem for the spectral parameter  $H_{\text{eff}}$  of the operator sheaf  $(\mathcal{H}_0 - BH_{\text{eff}})$ ,

$$\left( \mathcal{H}_0 \left( x, p, y, -i \frac{\partial}{\partial y}, t \right) - BH_{\text{eff}}(x, p, t) \right) \chi_0(x, p, y, t) = 0,$$

and the following equation for the corrections  $\chi_1$  and  $L_1$ :

$$\begin{aligned} \left( \mathcal{H}_0 \left( x, p, y, -i \frac{\partial}{\partial y}, t \right) - BH_{\text{eff}}(x, p, t) \right) \chi_1 = F_1 - \mathcal{H}_1 \chi_0 + B\chi_0 L_1, \quad F_1 = \hat{\mathcal{D}}\chi_0 \quad (4.17) \\ \hat{\mathcal{D}} = iB \frac{\partial}{\partial t} + i \sum_j \left[ \frac{\partial \mathcal{H}_0}{\partial p_j} \frac{\partial}{\partial x^j} - B \frac{\partial H_{\text{eff}}}{\partial x^j} \frac{\partial}{\partial p_j} \right] = iB \frac{d}{dt} + i \sum_j \frac{\partial(\mathcal{H}_0 - BH_{\text{eff}})}{\partial p_j} \frac{\partial}{\partial x^j}. \end{aligned}$$

We assume that the chosen spectral parameter  $H_{\text{eff}}(x, p, t)$  is nondegenerate, so  $\chi_0$  is a vector with five components  $\{\chi_{0j}\}$ ,  $j = 1, \dots, 5$ . Then the solution of the problem for the operator sheaf has the form

$$\begin{cases} \chi_{01} = i \frac{p_1}{p^2} \frac{\partial w(y, x, \alpha)}{\partial y}, \\ \chi_{02} = i \frac{p_2}{p^2} \frac{\partial w(y, x, \alpha)}{\partial y}, \\ \chi_{03} = w(y, x, \alpha), \\ \chi_{04} = i \frac{\partial \rho_0}{\partial y} \frac{w(y, x, \alpha)}{\Lambda}, \\ \chi_{05} = -i \rho_0 \frac{\Lambda}{p^2} \frac{\partial w(y, x, \alpha)}{\partial y}. \end{cases} \quad (4.18)$$

Here  $\Lambda = \langle U, p \rangle - H_{\text{eff}}(x, p)$ ,  $\alpha = \Lambda^2/p^2$ ,  $p^2 = p_1^2 + p_2^2$ ,  $w(y, x, \alpha)$  is an eigenfunction of the problem

$$\frac{1}{\rho_0(y, x)} \frac{\partial}{\partial y} \rho_0(y, x) \frac{\partial}{\partial y} w(y, x, \alpha) + \frac{\omega_0^2(y, x)}{\alpha} w(y, x, \alpha) = \varkappa(x, \alpha) w(y, x, \alpha),$$

and  $H_{\text{eff}}(x, p, t)$  is a solution of the algebraic equation

$$\varkappa \left( x, \frac{(\langle U, p \rangle - H_{\text{eff}}(x, p))^2}{p^2} \right) = p^2.$$

We choose an eigenvalue  $\varkappa$  and consider the corresponding function  $H_{\text{eff}}(x, p)$ . In general, this function is multi-valued; we fix one of its branches and assume that this branch is a smooth function of  $x, p$ .

The first correction  $L_1$  is found from the solvability condition for Equation (4.17). Its right-hand part must be orthogonal to the kernel of the adjoint operator  $(\mathcal{H} - BH_{\text{eff}})^*$ . We denote a function from its kernel by  $\chi_0^*$ . Then the first correction to the effective Hamiltonian is

$$L_1(x, p, t) = \frac{1}{\langle \chi_0^*, B\chi_0 \rangle} \left\langle \chi_0^*, \left[ \mathcal{H}_1 - iB \frac{d}{dt} - i \sum_j \frac{\partial(\mathcal{H}_0 - BH_{\text{eff}})}{\partial p_j} \frac{\partial}{\partial x^j} \right] \chi_0 \right\rangle_y.$$

To determine  $\chi_0^*$ , we note that the construction of the operator adjoint to  $(\mathcal{H}_0 - BH_{\text{eff}})$  is equivalent to the replacement  $|g\rangle \leftrightarrow -\partial\rho_0/\partial y$ . This gives

$$\chi_{0k}^* = \chi_{0k}, \quad k = 1, 2, 3, 5, \quad \chi_{04}^* = -i|g| \frac{w(y, x, \alpha)}{\Lambda}.$$

Using these relations, we obtain

$$\langle \chi_0^*, B\chi_0 \rangle_y = \frac{1}{p^2} \int \rho_0 \left| \frac{\partial w}{\partial y} \right|^2 dy + \int \rho_0 |w|^2 dy + \int \frac{\rho_0 \omega_0^2}{\Lambda^2} |w|^2 dy, \quad (4.19)$$

$$\begin{aligned} \langle \chi_0^*, \mathcal{H}_1 \chi_0 \rangle_y &= -\frac{i}{p^4} \sum_{j,k=1}^2 \frac{\partial U_j}{\partial x_k} p_j p_k \int \rho_0 \left| \frac{\partial w}{\partial y} \right|^2 dy - i \frac{\Lambda}{p^4} \langle p, \nabla f \rangle \\ &\times \left( \int \frac{\partial \bar{w}}{\partial y} \frac{\partial}{\partial y} \left( \rho_0 \frac{\partial w}{\partial y} \right) dy + c.c. \right) - i \frac{1}{p^2 \Lambda} \int \left\langle p, \nabla \rho_0 - \nabla f \frac{\partial \rho_0}{\partial y} \right\rangle \bar{w} \frac{\partial \rho_0}{\partial y} \frac{\partial w}{\partial y} dy + \frac{i}{p^2} \langle U, \nabla f \rangle \\ &\times \int \rho_0 \frac{\partial \bar{w}}{\partial y} \frac{\partial^2 w}{\partial y^2} dy + i \langle U, \nabla f \rangle \int \rho_0 \bar{w} \frac{\partial w}{\partial y} dy - i \langle U, \nabla f \rangle \frac{|g|}{\Lambda^2} \int \bar{w} \frac{\partial}{\partial y} \left( \frac{\partial \rho_0}{\partial y} w \right) dy. \end{aligned} \quad (4.20)$$

Using formulas (4.19–4.20) we can calculate the first correction  $L_1$ . We will not give here the explicit formula for  $L_1$  in the general case because of its awkward nature.

#### 4.4. ELECTROMAGNETIC WAVEGUIDES, INTEGRAL OPTICS, SURFACE GRAVITY WATER WAVES AND SHELLS

Electromagnetic-wave propagation in waveguides is described by the wave equation containing the second time-derivative. In the two-dimensional case, we have a situation similar to that considered in Section 2.2. One can easily generalize the scheme of Section 3 to this situation. The change consists in the following: instead of  $i\mu\psi_t$ , one must write the second time-derivative  $\mu^2\psi_{tt}$  in the left-hand side of (3.7). The same change allows one to consider three-dimensional waveguide problems. But now it is possible to consider waves in thin films (integral optics) or in thin tubes. The stationary variant of such equations is the Helmholtz equation

$$(\Delta + k^2 n(x))\Psi = 0 \quad (4.21)$$

with the refractive index  $n(x)$  and, *e.g.*, Dirichlet conditions  $\Psi = 0$  on the boundary of the film or the tube. The parameter  $\mu$  characterizes the ratio between the transverse and longitudinal dimensions of the waveguide; one can apply the adiabatic approximation if the boundary of the waveguide changes slowly. Maslov [55] considered problems of this type and constructed asymptotic solutions predicting the possibility of creating one-mode resonators by means of the waveguide geometry. Later on, problems of this type were considered in more general situations in optics and quantum mechanics (see, *e.g.*, [31–36, 56–59]).

The consideration of the Helmholtz equation is very similar to that of the stationary Schrödinger equation. In what follows, we consider the Schrödinger equation in a quantum waveguide in a more complicated situation.

More complicated examples similar to planar waveguides (thin films) lead to problems on wave propagation in shells. Instead of the wave equations, one must consider the Lamé equations in the theory of elasticity. The operator separation of variables can also be used in problems of this kind, but the study of these is far beyond the scope of this paper.

A more exotic example of operator separation of variables is given by the theory of surface gravity water waves over an uneven bottom (see, *e.g.*, [60]). Actually, this is the linearization of the problem with a free boundary and the *ansatz* (3.5) was first used in this situation [11]. The operator approach is discussed in detail in [11, 17, 18, 61], so we do not consider this problem here.

#### 4.5. NANOPHYSICS: WAVE PROPAGATION IN NANOFILMS

As far as adiabatic problems are concerned the two subsequent examples (quantum waves in nanofilms and nanotubes) are probably the simplest. An interest in these problems has arisen recently because of the enormous progress in nanotechnology. It seems that most of the results described below, as well as many recent mathematical results (*e.g.*, [31–36, 57–59]), have appeared only recently, because there was no keen physical interest in the corresponding problems before. Now the question is how to study concrete applied problems. Needless to say that the representation of the solution in a form appropriate for practical analysis is an additional and sometimes nontrivial problem (even in the case of nanofilms and nanotubes with simple structure, *e.g.*, without branching). So below we discuss some specific properties concerning quantum waveguides, present the effective equation of adiabatic (longitudinal) motion in thin films and tubes, and briefly touch upon only a few possible applications of the general theory to problems of quantum-waves in nanotubes with spin taken into account. The results of this subsection represent the particular case of the general results concerning quantum-wave propagation in thin films taking spin into account. These more general results were obtained in collaboration with Brüning [62].

Thin crystalline films of width  $\sim 10\text{nm}$  (a few monoatomic layers), synthesized recently, give a more complicated example of a quantum waveguide. Such a film is a waveguide for a quasi-particle with charge  $e$  propagating along the film, and we can affect this particle by means of an external electromagnetic field. In reality, a quasi-particle has spin, but we shall not consider spin effects for nanofilms.

The nanofilm width  $d_0 \sim 1\text{ nm}$  ( $10\text{ \AA}$ ) is comparable with a de Broglie wavelength of  $\lambda = 2\pi/k_F \sim 1\text{ nm}$  of an electron with an energy of the order of the Fermi energy  $\varepsilon_F \sim 1\text{ eV}$ . This circumstance leads to the following effect of “dimensional quantization” of low-dimensional systems: the domain of the wave-function localization in a normal direction to the film has dimensions  $\sim \lambda$ , and the energy corresponding to the motion in this direction is quantized. Therefore, the total three-dimensional problem of describing the quantum states can be divided into several reduced problems (on “subbands of dimensional quantization”) already with two-dimensional quantum effective Hamiltonians (along the film surface), which, in the end, allows one to obtain a sufficiently explicit description of these states by using asymptotic formulas.

The film boundaries play an important role in future constructions. A natural idea is to simulate the boundaries of the film by means of the Dirichlet conditions or “rigid walls” for the wave function. But it is more convenient to simulate by using so-called “soft walls.” Boundaries of this type are related to the physical mechanism of confinement of electrons

near the physical film. The confinement appears as a result of the electrostatic interaction between the film and the quasi-particle. One usually simulates this interaction by introducing a confinement potential  $v_{\text{int}}$  in a direction normal to the film. The potential  $v_{\text{int}}$  increases very fast near the imaginary boundaries of the film (the “walls”). Thus, the wave function decays very fast outside the film and the confinement potential  $v_{\text{int}}$  replaces the “rigid” walls simulated by the Dirichlet conditions. From a “mechanical” point of view the confinement potential represents the interaction with imaginary walls. The same idea is used when simulating nanotubes. We shall present the corresponding formulas somewhat later.

The effective dynamics of quantum states in the approximation of the strong coupling method is determined by the Schrödinger equation:

$$i\hbar\Psi_t = \widehat{\mathcal{H}}\Psi, \quad \widehat{\mathcal{H}} = \frac{\widehat{\mathbf{P}}^2}{2m} + v_{\text{int}}(r) + v_{\text{ext}}(\mathbf{r}, t), \quad (4.22)$$

where  $\widehat{\mathbf{P}} = -i\hbar\nabla - (e/c)\mathbf{A}(\mathbf{r}, t)$ ,  $e = -e_0$  is the charge of electron,  $m$  is the effective mass of quasi-particle,  $c$  is the velocity of light, and  $(v_{\text{ext}}(\mathbf{r}, t), \mathbf{A})$  are the potentials of external electromagnetic field. We shall consider a space-uniform time-dependent magnetic field  $\mathbf{H} = \mathbf{H}(t)$ .

The characteristic value of the transverse energy  $\varepsilon_{\perp}$  in the tube can be found from the uncertainty relation: since the “transverse” momentum is  $\sim \hbar/d_0$ , we have  $\varepsilon_{\perp} \sim \hbar^2/(md_0^2)$ . Let us introduce the characteristic “longitudinal” length  $l_0$ . Depending on the problem considered,  $l_0$  can be, for instance, the radius of curvature of the film or the radius of the solution localization area, etc. We assume that  $l_0 \gg d_0$ . We introduce the magnetic length  $l_M = \sqrt{\hbar c/(e|\mathbf{H}|)}$ , the magnetic field quantum  $\Phi_0 = 2\pi\hbar c/e$ , and the dimensionless magnetic field as the number of magnetic flux quanta passing through the characteristic area  $l_0 d_0$ :  $\mathbf{H}' = l_0 d_0 / l_M^2 \cdot \mathbf{H} / |\mathbf{H}| = 2\pi l_0 d_0 \cdot \mathbf{H} / \Phi_0$ . We introduce the new variables  $\mathbf{r}' = \mathbf{r} / l_0$ , the dimensionless time  $t' = t / T$ ,  $T = md_0 l_0 / \hbar$ , the dimensionless potentials  $v'_{\text{int}} = v_{\text{int}} / \varepsilon_{\perp}$ ,  $v'_{\text{ext}} = v_{\text{ext}} / \varepsilon_{\perp}$ ,  $\mathbf{A}' = ed_0(\hbar c)^{-1}\mathbf{A}$ , and the dimensionless constant  $\alpha' = \hbar\alpha / d_0^2$  and divide both sides of (4.22) by the energy of transverse motion  $\varepsilon_0$ . Below, we shall omit the primes. Then the equation describing the motion of a quantum particle (or a quasi-particle) in a quasi-two-dimensional crystal takes the form

$$i\mu\Psi_t = \widehat{\mathcal{H}}\Psi, \quad \widehat{\mathcal{H}} = 1/2(-i\mu\nabla - \mathbf{A})^2 + v_{\text{int}}(\mathbf{r}) + v_{\text{ext}}(\mathbf{r}, t). \quad (4.23)$$

The fact that we consider the last equation in a film is determined by the boundary conditions. We shall assume that the film is determined by some smooth surface  $\Gamma$ . This means that Equation (4.23) holds and the boundary conditions are formulated in some neighborhood of  $\Gamma$ . It is convenient to use special curvilinear coordinates for the description of these conditions, as well as for all future investigations.

#### 4.5.1. Curvilinear coordinates

By  $x = (x^1, x^2)$  we denote the (dimensionless) local coordinates on the surface  $\Gamma$ ; then each point  $\mathbf{r}$  in a neighborhood of  $\Gamma$  can be determined by three values  $(x^1, x^2, y)$ , where  $y$  is the distance between the point  $\mathbf{r}$  and its projection  $R(x) \in \Gamma$ . Then we have

$$\mathbf{r} = \mathbf{R}(x) + y\mathbf{n}(x),$$

where, as above,  $\mathbf{n}(x)$  is a unit normal vector on  $\Gamma$ . Note that, in general, the coordinates  $x^1, x^2$  are not orthogonal, but always  $\langle \mathbf{n}, \mathbf{n} \rangle = 1$ ,  $\langle \mathbf{n}, \partial_i \mathbf{R} \rangle = 0$ ,  $i = 1, 2$ . Thus the metric tensor is

$$G_{ab} = \left\| \begin{array}{cc} \gamma_{ij} & 0 \\ 0 & 1 \end{array} \right\|, \quad G = \det G_{ab}, \quad a, b = 1, 2, 3, \quad (4.24)$$

where  $\gamma_{ij} = \langle \partial_i \mathbf{r}, \partial_j \mathbf{r} \rangle$ ,  $\gamma = \det \gamma_{ij}$ ,  $i, j = 1, 2$ , and  $G = \gamma$ . Now let us present the components of the vector potential  $\mathbf{A}$  in the coordinates  $(x^1, x^2, y)$ . We choose the symmetric form of the vector potential  $\mathbf{A} = 1/2[\mathbf{H}, \mathbf{r}]$ . Hence the vector potential satisfies the Lorentz gauge:  $\partial A^a / \partial r^a = 0$ . From now on, it is convenient to use the Einstein notation and the summation rule.

#### 4.5.2. Soft and rigid walls

Using curvilinear coordinates, one can consider an “empty” film with “rigid” walls:  $v_{\text{int}} = 0$ ,  $\Psi|_{\partial\Omega} = 0$  (the Dirichlet condition) or a film with “soft” walls:  $v_{\text{int}} \neq 0$ ,  $\Psi(x, y) \in L_2(y)$  at each  $x$ . However, the last definition requires  $v_{\text{int}}(x, y)$  to be identically defined in the entire  $\mathbb{R}^3$ . The last condition is too strong, since  $\Psi(x, y)$  is exponentially small for  $y \gg \mu$  and any conditions on the function  $\Psi$  in this region affect its behavior negligibly. To be definite, in what follows, we assume that  $\Psi(x, y)|_{\partial\Omega} = 0$ . The “empty” film with “rigid” walls can be considered as the limit of soft walls described by the potential rapidly increasing near the boundary. As an example, let us consider the potential  $v_{\text{int}}(x, y) = (y'/D(x))^{2m}$ ,  $y' = y/\mu$ ,  $m > 0$ . As  $m \rightarrow \infty$ , we have  $v_{\text{int}}(x, y < d(x)) \rightarrow 0$  and  $v_{\text{int}}(x, y > d(x)) \rightarrow \infty$ .

#### 4.5.3. Operator-valued symbol in a nanofilm

It is well known that the use of the function  $\Psi' = \Psi G^{1/4}$  instead of  $\Psi$  can significantly simplify the corresponding calculations. Substituting the function  $\Psi = G^{-1/4} \Psi'$  in (4.23), we obtain the following equation for the function  $\Psi'$ :

$$i\mu \Psi'_i = \widehat{\mathcal{H}}' \Psi', \quad \widehat{\mathcal{H}}' = G^{1/4} \widehat{\mathcal{H}} G^{-1/4}. \quad (4.25)$$

Using the formula  $G^{1/4} \Delta G^{-1/4} = G^{ab} \partial_a \partial_b + G_{,a}^{ab} \partial_b + G^{-1/4} \partial_a (G^{1/2} G^{ab} \partial_b (G^{-1/4}))$ , we obtain

$$\begin{aligned} \widehat{\mathcal{H}}' = & \frac{1}{2} G^{ab} \hat{p}_a \hat{p}_b - \frac{i\mu}{2} G_{,a}^{ab} \hat{p}_b - \frac{\mu^2}{2} \frac{1}{G^{1/4}} \partial_a \left[ G^{1/2} G^{ab} \partial_b \left( \frac{1}{G^{1/4}} \right) \right] \\ & - G^{ab} A_a \hat{p}_b - \frac{i\mu}{4} G^{ab} A_a \partial_b (\log G) + \frac{1}{2} G^{ab} A_a A_b + v_{\text{ext}}(x, y, t) + v_{\text{int}}(x, y/\mu). \end{aligned}$$

We want to study solutions to Equation (4.25) that feature only a few oscillations in the transverse direction. From a physical point of view it is clear that, in general, the nontrivial behavior of such solutions should be determined by two-dimensional effective equations of adiabatic motion (3.7) on the surface  $\Gamma$  in a neighborhood of the physical film. Recall that our goal is to find these reduced equations corresponding to solutions with different numbers of transverse oscillations. As we have different scales in the transverse and longitudinal direction, it is natural to use the variable  $y' = y/\mu$  instead of  $y$ . To simplify the notation, we omit the prime. Then the operator  $\widehat{\mathcal{H}}'$  in (4.25) is

$$\begin{aligned} \widehat{\mathcal{H}}' = & \frac{\gamma^{ij}}{2} (\hat{p}_i \hat{p}_j - 2A_i \hat{p}_j + A_i A_j) + \frac{1}{2} (\hat{p}_y^2 - 2A_y \hat{p}_y + A_y^2) + v_{\text{ext}}(\mathbf{r}, t) + v_{\text{int}}(x, y) \\ & - \frac{i\mu}{2} \gamma_{,i}^{ij} \hat{p}_j - \frac{i\mu}{4} \gamma^{ij} A_i \partial_j (\log \gamma) - \frac{i}{4} A_y \partial_y (\log \gamma) \\ & - \frac{\mu^2}{2} \frac{1}{\gamma^{1/4}} \partial_i \left[ \gamma^{1/2} \gamma^{ij} \partial_j \left( \frac{1}{\gamma^{1/4}} \right) \right] - \frac{1}{2} \frac{1}{\gamma^{1/4}} \partial_y \left[ \gamma^{1/2} \partial_y \left( \frac{1}{\gamma^{1/4}} \right) \right], \end{aligned} \quad (4.26)$$



where  $A_i = \langle \partial_i \mathbf{r}, \mathbf{A} \rangle$  and  $A_y = \langle \mathbf{n}, \mathbf{A} \rangle$ . Equation (4.25), with the Hamiltonian determined by formula (4.26), is the object of our future study.

Using these formulas, we find the first and second terms of the expansion of the symbol of operator  $\hat{\mathcal{H}}'$ :

$$\mathcal{H}'_0 \left( x, p, y, -i \frac{\partial}{\partial y}, t \right) = \frac{1}{2} g^{ij} \mathcal{P}_i \mathcal{P}_j + \frac{1}{2} \hat{\mathcal{P}}_y^2 + v_{\text{ext}}(\mathbf{R}(x), t) + v_{\text{int}}(x, y), \quad (4.27)$$

$$\begin{aligned} \mathcal{H}'_1 \left( x, p, y, -i \frac{\partial}{\partial y}, t \right) = & \frac{1}{2} y \gamma_1^{ij} \mathcal{P}_i \mathcal{P}_j - y g^{ij} \mathcal{P}_i A_j^1 + \langle \nabla v_{\text{ext}}(\mathbf{R}(x), t), y \mathbf{n} \rangle \\ & - i \left( \frac{1}{2} g_{,i}^{ij} p_j + \frac{1}{4} g^{ij} A_i^0 \partial_j (\log g) + \frac{1}{4} A_y^0 [\partial_y (\log \gamma)]_{y=0} \right), \end{aligned} \quad (4.28)$$

where  $p = (p_1, p_2)$ ,  $\mathbf{A} = \mathbf{A}_0 + \mu y \mathbf{A}_1$ ,  $\mathbf{A}_0 = 1/2[\mathbf{H}, \mathbf{R}]$ ,  $\mathbf{A}_1 = 1/2[\mathbf{H}, \mathbf{n}]$ ,  $A_i = A_i^0 + \mu y A_i^1 + O(\mu^2)$ ,  $A_i^0 = \langle \partial_i \mathbf{R}, \mathbf{A}_0 \rangle$ ,  $A_i^1 = \langle \partial_i \mathbf{R}, \mathbf{A}_1 \rangle + \langle \partial_i \mathbf{n}, \mathbf{A}_0 \rangle$ ,  $A_y = A_y^0 + \mu y A_y^1 + O(\mu^2)$ ,  $A_y^0 = \langle \mathbf{n}, \mathbf{A}_0 \rangle$ ,  $A_y^1 = \langle \mathbf{n}, \mathbf{A}_1 \rangle = 0$ ,  $\mathcal{P}_i = p_i - A_i^0$ , and  $\hat{\mathcal{P}}_y = p_y - A_y^0$ .

To describe the so-called slow modes, we need to compute  $\mathcal{H}'_2$  under the assumption that  $\mathcal{P}_i = 0$ ,  $v_{\text{ext}} = 0$ , and  $\partial \mathbf{H} / \partial t = 0$ . We obtain

$$\mathcal{G}(x) = -\frac{(\varkappa_1 - \varkappa_2)^2}{8} - \frac{1}{2g^{1/4}} \partial_i \left[ g^{1/2} g^{ij} \partial_j \left( \frac{1}{g^{1/4}} \right) \right]. \quad (4.29)$$

This term is independent of  $y$  and  $\hat{p}_y$  and contains only geometric characteristics of the embedding (the first summand) and the limiting manifold (the second summand). We call it a *geometric potential*.

#### 4.5.4. Effective Hamiltonians of longitudinal motion

Now we present  $\chi_0^v$  and the effective ‘‘adiabatic’’ Hamiltonians  $H_{\text{eff}}^v$ . The index  $v$  enumerates the Hamiltonians  $H_{\text{eff}}^v$  which, in our problem, is called the effective adiabatic Hamiltonian on the  $v$ -th subband of the size quantization. Substituting the function  $\chi_0^v = \exp(iy \langle \mathbf{n}, \mathbf{A}_0 \rangle) w^v$  in (3.12) with  $\mathcal{H}_0 = \mathcal{H}'_0$ , we obtain

$$H_{\text{eff}}^v(p, x, t) = \frac{1}{2} g^{ij} \mathcal{P}_i \mathcal{P}_j + v_{\text{ext}}(\mathbf{R}(x), t) + \varepsilon_{\perp}^v(x), \quad \chi_0 = \exp(iy \langle \mathbf{n}, \mathbf{A}_0 \rangle) w^v. \quad (4.30)$$

where  $w^v(x, y)$  and  $\varepsilon_{\perp}^v(x)$  are the respective eigenfunction and eigenvalue of the following problem:

$$\left( -\frac{1}{2} \frac{\partial^2}{\partial y^2} + v_{\text{int}}(x, y) \right) w^v(x, y) = \varepsilon_{\perp}^v(x) w^v(x, y), \quad w^v(x, Y_1(x)) = w^v(x, Y_2(x)) = 0. \quad (4.31)$$

It is well known that the spectrum of this problem is nondegenerate, thus the symbols  $L$  and  $\chi^v$  are scalar functions. For the model potential  $v_{\text{int}}(x, y) = (y/D(x))^{2m}$ ,  $m > 0$  considered in Section 4.5.2, we obtain  $\varepsilon_{\perp}^v(x) = (d(0)/d(x))^2 \varepsilon_{\perp}^v(0)$ , where  $d(x) = D(x)^{\frac{m}{m+1}} d(0)$  is the dispersion of the state with energy  $\varepsilon_{\perp}^v(x)$ . Assuming that the width of the film is proportional to  $d(x)$ , we conclude that  $D(x)^{\frac{m}{m+1}}$  is the coefficient of homothety. As  $m \rightarrow \infty$ , this coefficient tends to  $D(x)$ . So we obtain the natural result stating that, in the model of an empty film with rigid walls, the width of the film is equal to the distance between the walls.

Let us present the first correction  $\mu L_1$  in an expansion of the symbol of the effective Hamiltonian of longitudinal motion. It is given by formula (3.16).

Using the formula for  $\chi_0^v$  and the expansion of the gauge condition  $\partial_i (\gamma^{ij} A_j) + 1/2 \gamma^{ij} A_i \partial_j (\log \gamma) + \partial_y A_y + 1/2 A_y \partial_y (\log \gamma) = 0$  with respect to  $y = \mu y'$ , we may easily obtain

the relations

$$\langle w^\nu, \partial_j w^\nu \rangle_y = 0, \quad \left\langle \chi_0^\nu, \frac{\partial \chi_0^\nu}{\partial t} \right\rangle_y = iY \left\langle \mathbf{n}, \frac{\partial \mathbf{A}_0}{\partial t} \right\rangle, \quad \left\langle \chi_0^\nu, \frac{\partial H_{\text{eff}}}{\partial p_j} \frac{\partial \chi_0^\nu}{\partial x^j} \right\rangle_y = iY g^{ij} \mathcal{P}_i \partial_j \langle \mathbf{n}, \mathbf{A}_0 \rangle,$$

where  $Y = \langle \chi_0^\nu, y \chi_0^\nu \rangle_y$ , and

$$Y g^{ij} \mathcal{P}_i (\partial_j \mathbf{R}, \mathbf{A}_1) = -Y g^{ij} \mathcal{P}_i \langle \mathbf{n}, \partial_j \mathbf{A}_0 \rangle = 1/2 \langle \mathbf{H}, \Lambda \rangle, \\ \partial_i (g^{ij} A_j^0) + \frac{1}{2} g^{ij} A_i^0 \partial_j (\log g) + A_y^0 [\partial_y (\log \gamma)]_{y=0} = 0, \quad g_{,i}^{ij} p_j - \partial_i (g^{ij} A_j^0) = \partial_i (g^{ij} \mathcal{P}_j). \quad (4.32)$$

From this, we find

$$L_1 = -Y \alpha_j^i g^{jk} \mathcal{P}_i \mathcal{P}_k - \langle \mathbf{E}(\mathbf{R}(x), t), Y \mathbf{n} \rangle - \langle \mathbf{H}, \Lambda \rangle - \frac{i}{2} \partial_i (g^{ij} \mathcal{P}_j), \quad (4.33)$$

where  $\Lambda = [Y \mathbf{n}, \mathcal{P}]$ ,  $\mathcal{P} = g^{ij} \mathcal{P}_i \partial_j \mathbf{R}$ , and  $\mathbf{E} = -\nabla v_{\text{ext}} - T(\partial \mathbf{A}_0 / \partial t)$ . We shall see below that the correction  $L_2$  is important in the construction of the leading term of the asymptotic solution to the effective equation of adiabatic (longitudinal) motion only under the assumptions  $\mathcal{P}_i = 0$ ,  $v_{\text{ext}} = 0$ , and  $\partial \mathbf{H} / \partial t = 0$ . In this case, it coincides with the ‘‘geometric’’ potential  $\mathcal{G}(x)$  (4.29).

#### 4.6. NANOPHYSICS: WAVE DYNAMICS IN NANOTUBES

##### 4.6.1. *The Pauli operator*

Lengthy molecules consisting of a great many atoms situated on cylinder-type spatial surfaces are called *nanotubes* [63–70]. The surface of such tubes can have some additional internal torsion. The nanotube diameter  $d_0 \sim 1$  nm (10 Å) is comparable with the de Broglie wavelength  $\lambda = 2\pi/k_F \sim 1$  nm of an electron with energy of the order of the Fermi energy  $\varepsilon_F \sim 1$  eV, and the nanotube characteristic length  $l_0$  is significantly larger than  $d_0$ .

In the approximation of the strong coupling method, the wave functions in nanotubes are determined by the nonrelativistic one-particle Hamiltonian, *i.e.*, by the Pauli operator with the spin-orbit interaction taken into account:

$$\widehat{\mathcal{H}} = \frac{\widehat{\mathbf{P}}^2}{2m} + v_{\text{int}}(\mathbf{r}) + v_{\text{ext}}(\mathbf{r}, t) - \frac{e\hbar}{2mc} \langle \boldsymbol{\sigma}, \mathbf{H} \rangle + \widehat{\mathcal{H}}_{\text{SO}}, \quad \widehat{\mathbf{P}} = -i\hbar \nabla - \frac{e}{c} \mathbf{A}(\mathbf{r}, t). \quad (4.34)$$

Here  $\mathbf{r} \in \mathbb{R}^3$  is the radius vector of a point in a neighborhood of the tube,  $\widehat{\mathcal{H}}_{\text{SO}}$  is the operator of interaction of the electron spin with the electric field of the crystal [71]:  $\widehat{\mathcal{H}}_{\text{SO}} = \alpha \langle \boldsymbol{\sigma}, [\nabla v_{\text{int}}, \widehat{\mathbf{P}}] \rangle$ , and  $\alpha$  is the constant of spin-orbit interaction. This Hamiltonian differs from that in a nanofilm (4.22) only by the presence of terms describing spin effects. Thus, all the notation is the same.

In this section we consider some of results published in [72–74].

##### 4.6.2. *Curvilinear coordinates in tubes*

As in the case of thin films, it is convenient to perform all arguments by using a special system of curvilinear coordinates. We assume that the tube axis (the curve)  $\gamma$  is given by the equation  $\mathbf{r} = l_0 \mathbf{R}(x)$ ,  $\mathbf{r} \in \mathbb{R}^3$ , where  $\mathbf{R}(x)$  is a smooth vector function and  $x \in \mathbb{R}$  is a natural parameter on  $\gamma$  (the tube length is counted from a certain point  $x^*$ ),  $|\partial_x \mathbf{R}(x)| = 1$ ,  $\partial_x = \partial / \partial x$ . If  $|\partial_x^2 \mathbf{R}| \neq 0$ , the Frenet trihedron can be determined. The curvature  $k(x) = |\partial_x^2 \mathbf{R}|$  and the torsion  $\varkappa(x)$  of the curve  $\gamma$  are connected by the Frenet trihedron  $\{\partial_x \mathbf{R}, \mathbf{n} = \partial_x^2 \mathbf{R} / |\partial_x^2 \mathbf{R}|, \mathbf{b} = [\partial_x \mathbf{R}, \mathbf{n}]\}$  at each point  $x$  by the formulas  $\partial_x \mathbf{n} = -\varkappa \mathbf{b} - k \partial_x \mathbf{R}$  and  $\partial_x \mathbf{b} = \varkappa \mathbf{n}$ .

By  $\Pi(x)$  we denote the plane intersecting the tube axis at the point  $\mathbf{R}(x)$  orthogonally to the axis; the section of the tube by this plane (the area in  $\Pi(x)$ ) is denoted by  $\Omega(x)$ ,

the boundary of  $\Omega(x)$  by  $\partial\Omega(x)$ . Then the tube is the union of the areas  $\Omega(x)$ , and its boundary is the union of  $\partial\Omega(x)$ . The “physical meaning” of the boundary  $\partial\Omega(x)$  and of the boundary conditions will be discussed later. We introduce dimensionless coordinates  $(x, y_1, y_2)$  determined by the relations  $\mathbf{r} = l_0\mathbf{R}(x) + \mathbf{y}$ ,  $\mathbf{y} = d_0y_1\mathbf{n}_1(x) + d_0y_2\mathbf{n}_2(x)$ , where  $\{\mathbf{n}_1(x), \mathbf{n}_2(x)\}$  is the basis in the plane  $\Pi(x)$ .

If we put  $\mathbf{n}_1 = \mathbf{n}$ ,  $\mathbf{n}_2 = \mathbf{b}$ , then the coordinates thus introduced will be nonorthogonal. It is convenient to introduce orthogonal coordinates (see [75, 76]). First, let  $\{\mathbf{n}_1(x), \mathbf{n}_2(x)\}$  be a certain orthonormal basis in the plane  $\Pi(x)$  smoothly depending on  $x$  (in general, this basis does not coincide with  $\mathbf{n}, \mathbf{b}$ ); and let  $\theta(x)$  be the angle between the vectors  $\mathbf{n}$  and  $\mathbf{n}_1$ . Then, along with the torsion  $\varkappa$ , we can introduce an “effective torsion”  $\varkappa_{\text{eff}} = -(\partial_x \mathbf{n}_1, \mathbf{n}_2) = \varkappa - \partial_x \theta$ . Choosing the angle  $\theta(x)$  (along with  $\{\mathbf{n}_1(x), \mathbf{n}_2(x)\}$ ) so that  $\partial_x \theta = \varkappa$ , we let  $\varkappa_{\text{eff}}$  be zero. The coordinates thus constructed are orthogonal (around the tube axis, where they are specified). The components of the metric tensor  $g_{ij}$ ,  $i, j = \{x, y_1, y_2\}$  in these coordinates are determined as follows:  $g_{00} = G = (1 - k(\mathbf{y}, \mathbf{n}))^2$ ,  $g_{11} = g_{22} = 1$ , and  $g_{ij} = 0, i \neq j$ . Everywhere below we shall use these coordinates. All formulas obtained below are valid in the case of a straight axis if we set  $k(x) = 0$  and  $\varkappa(x) = 0$ . If  $k(x) \neq 0$ , then  $y_1$  and  $y_2$  are the coordinates only in the area where  $1 - k(\mathbf{y}, \mathbf{n}) > 0$ . It follows from the considerations about the tube curvature given below that these coordinates are determined in the area of the tube axis under study.

#### 4.6.3. Boundary conditions and geometry of nanotubes

As in the case of a nanofilm, the “surface” of a nanotube can be simulated by “rigid” and “soft” walls. The rigid walls are determined by the imaginary surface of the tube and the Dirichlet conditions on this surface. The soft walls are simulated by an appropriate choice of the crystal potential  $v_{\text{int}}(y, x)$  rapidly increasing while approaching the imaginary surface of the tube and creating a potential well where the electron wave function is localized. Outside this well, the wave function is exponentially small. We shall consider tubes whose cross-section by the plane  $\Pi(x)$  rotates with respect to the basis  $\{\mathbf{n}_1(x), \mathbf{n}_2(x)\}$  in which the metric tensor is diagonal, and simultaneously expands in the plane  $x = \text{const}$  with respect to the point  $\mathbf{R}(x)$ . We define the tube’s chirality as follows: we fix a cross-section  $\Omega_{x^*}$  for some  $x^* \in \gamma$  and assume that, at a point  $x \neq x^*$ , the cross-section  $\Omega_x$  is obtained from  $\Omega_{x^*}$  by a turn through an angle  $\Phi(x)$  (i.e., through an “angle of internal torsion” with respect to the basis  $\{\mathbf{n}_1(x), \mathbf{n}_2(x)\}$ ) and by expanding by a factor  $D(x)$ .

The domain  $\Omega(x)$  can be introduced as a multiply connected domain, for example, in the form of a circular or an elliptic annulus. The adequacy of this representation depends on the form of the crystal potential in a given nanotube. If the domain  $\Omega(x)$  is simply connected, then, in the physical literature, such a nanotube is called a “quantum wire” [34, 35].

#### 4.6.4. Operator-valued symbol

The way of introducing dimensionless variables in a nanotube is the same as in the previous Example 4.5. It is convenient to pick out the factor  $G^{-1/4}$  from the wave function  $\Psi$ , where  $G$  is the determinant of the metric tensor in the variables  $(x, y_1, y_2)$ , i.e., to substitute  $\Psi = G^{-1/4}\Psi'$  in the original equation. Then the function  $\Psi'$  satisfies the equation  $i\mu\Psi'_t = \hat{\mathcal{H}}'\Psi'$ ,  $\hat{\mathcal{H}}'G^{1/4}\mathcal{H}G^{-1/4}$ . In what follows, we shall use the wave function  $\Psi'$  and the Hamiltonian  $\hat{\mathcal{H}}'$ . After some transformations, the quantum Hamiltonian  $\hat{\mathcal{H}}'$  takes the standard form (2.2) with the operator-valued symbol

$$\mathcal{H}' = \mathcal{H}'_0 + \mu\mathcal{H}'_1 + \mu^2(\mathcal{G}(x) + \tilde{\mathcal{H}}'_2) + O(\mu^3),$$

where

$$\begin{aligned}\mathcal{H}'_0 &= \frac{\mathcal{P}_0^2}{2} + v_{\text{ext}}(\mathbf{R}(x), t) + \sum_{j=1}^2 \frac{\widehat{\mathcal{P}}_j^2}{2} + v_{\text{int}}(x, y), \\ \mathcal{H}'_1 &= -1/2 \langle \partial_x \mathbf{R}, \mathbf{H} \rangle \hat{l} + ik/2 \langle \mathbf{n}, \mathbf{A}_0 \rangle + \left( k \langle \mathbf{y}, \mathbf{n} \rangle \mathcal{P}_0 - 1/2 \langle \mathbf{y}_\perp, \mathbf{H} \rangle \right) p \\ &\quad + \left\langle \nabla v_{\text{ext}}(\mathbf{R}(x), t) + 1/2 [\mathbf{A}_0, \mathbf{H}], \mathbf{y} \right\rangle - 1/2 \langle \boldsymbol{\sigma}, \mathbf{H} \rangle + \mu^{-1} \alpha \langle \boldsymbol{\sigma}, \hat{\mathbf{M}} \rangle,\end{aligned}\quad (4.35)$$

and we introduced the notation

$$\begin{aligned}\mathcal{P}_0 &= p - \langle \partial_x \mathbf{R}, \mathbf{A}_0 \rangle, \quad \widehat{\mathcal{P}}_j = -i\partial/\partial y_j - \langle \mathbf{n}_j, \mathbf{A}_0 \rangle, \quad j = 1, 2, \\ \hat{l} &= i(y_2 \partial/\partial y_1 - y_1 \partial/\partial y_2), \quad \mathbf{y}_\perp = [\mathbf{y}, \partial_x \mathbf{R}] = y_1 \mathbf{n}_2 - y_2 \mathbf{n}_1, \quad \mathbf{A}_0 = 1/2 [\mathbf{H}(t), \mathbf{R}(x)], \\ \hat{\mathbf{M}} &= \partial_x \mathbf{R} \left( \frac{\partial v_{\text{int}}}{\partial y_1} \widehat{\mathcal{P}}_2 - \frac{\partial v_{\text{int}}}{\partial y_2} \widehat{\mathcal{P}}_1 \right) + \mathbf{n}_1 \frac{\partial v_{\text{int}}}{\partial y_2} \mathcal{P}_0 - \mathbf{n}_2 \frac{\partial v_{\text{int}}}{\partial y_1} \mathcal{P}_0.\end{aligned}\quad (4.36)$$

For the symbol  $\mathcal{H}'_2$ , we present only its “geometric” part  $\mathcal{G}(x) = -k^2/8$ , the “remainder”  $\tilde{\mathcal{H}}'_2 = \mathcal{H}'_2 - \mathcal{G}$  is a polynomial with respect to the momentum  $\mathcal{P}_0$  and the components of the magnetic field  $\mathbf{H}(t)$  with zero constant term and with coefficients smoothly depending on  $(x, y)$ . In what follows, we shall see that the explicit form of this “remainder” is not necessary for the construction of the leading terms of asymptotic solutions to the effective equation of adiabatic (longitudinal) motion.

The boundary conditions (rigid and soft walls) defining the nanotube are similar to those in the case of a nanofilm. The corresponding change will be discussed somewhat later.

#### 4.6.5. Reduction to equations on the tube axis and the adiabatic Hamiltonian

Now we want to use the scheme of Section 3 and to find the symbol  $L$  of the effective equation of adiabatic motion (along the tube axis). This case is characterized by the fact that the reduced equation contains a single spatial variable. Thus, it is natural immediately to separate the factor  $\exp(i \int_{x^*}^x \langle \partial_x \mathbf{R}, \mathbf{A}_0 \rangle dx / \mu)$  in the wave function. This separation takes the extended momentum operator  $\hat{\mathcal{P}}$  into the “short” operator  $\hat{p} = -i\mu \partial/\partial x$  but, in the case of a magnetic field depending on time  $t$ , gives the correction  $\int_{x^*}^x \langle \partial_x \mathbf{R}, \partial \mathbf{A}_0 / \partial t \rangle dx$  to the effective potential. Next, because the function  $\Psi$  is a spinor and  $\mathcal{H}_0$  is a scalar operator, the true multiplicity of degeneration of the term determining the reduced equation is equal to  $2r$  (the definition of  $r$  is given later).

Taking these remarks into account, we present the solution  $\Psi$  of Equation (2.2) in the form

$$\Psi(x, y, t, \mu) = \hat{\chi}^\nu \left[ \exp \left( i \int_{x^*}^x \langle \partial_x \mathbf{R}, \mathbf{A}_0 \rangle dx / \mu \right) \psi^\nu \right], \quad \hat{\chi}^\nu = \chi^\nu \left( -i\mu \frac{\partial}{\partial x}, \frac{x}{\mu}, y, t, \mu \right), \quad (4.37)$$

where the symbol  $\chi^\nu(x, p, y, t, \mu) = \chi_0^\nu(x, p, y, t, \mu) + \mu \chi_1^\nu(x, p, y, t, \mu) + \dots$  of the (pseudo) differential operator  $\hat{\chi}^\nu(x, p, y, t, \mu)$  is a matrix function consisting of  $2r$  columns and 2 rows and  $\psi$  is a vector function with  $2r$  (interacting) components  $\psi^{vj}$  satisfying Equation (3.7). As was mentioned above, to construct the leading term of the asymptotic solution to this equation, we need only to have its *essential part*  $L_0^\nu(p, x) + \mu L_1^\nu(p, x) + \mu^2 \mathcal{G}(x)$ .

Equation (3.12) can be reduced to the equation

$$\left( -\frac{\Delta_y}{2} + v_{\text{int}}(x, y) \right) w^\nu = \varepsilon_\perp^\nu(x) w^\nu \quad (4.38)$$

by the substitutions  $\chi_0^\nu = \exp(i \langle \mathbf{y}, \mathbf{A}_0 \rangle) w^\nu$  and

$$H_{\text{eff}}^\nu = \frac{p^2}{2} + v_{\text{ext}}(\mathbf{R}(x), t) + \varepsilon_\perp^\nu(x) + \int_0^x \left\langle \partial_x \mathbf{R}(x'), \frac{\partial \mathbf{A}_0}{\partial t}(x', t) \right\rangle dx'. \quad (4.39)$$

Here  $\nu$  is just the number of the (classical) effective Hamiltonian (or the adiabatic term) which is also called the number of a *subband of dimensional quantization*. The eigenvalue  $\varepsilon_{\perp}^{\nu}(x)$  is the energy of the  $\nu$ th transverse mode at a point  $x$ . In contrast to the case of nanofilms, the eigenvalues  $\varepsilon_{\perp}^{\nu}$  (and hence the effective Hamiltonians) can be degenerate. The number  $r$ , which appeared above, is precisely their multiplicity. Generally speaking,  $r$  can depend on  $x$ , and in this case the effect called “the intersection of terms or effective Hamiltonians” can occur [77–80]. Here we assume that  $r$  is independent of  $x$ . Finally, we have

$$\begin{aligned} \chi_0^{\nu} &= \exp(i\langle \mathbf{y}, \mathbf{A}_0 \rangle) \| w_1^{\nu}, \dots, w_r^{\nu} \| \otimes E_s, \\ \| w_1^{\nu}, \dots, w_r^{\nu} \| \otimes E_s &= \left\| \begin{array}{cccc} w_1^{\nu}(x, y) & 0 & \cdots & w_r^{\nu}(x, y) & 0 \\ 0 & w_1^{\nu}(x, y) & \cdots & 0 & w_r^{\nu}(x, y) \end{array} \right\|, \end{aligned} \quad (4.40)$$

where  $\otimes$  is the tensor product of matrices and  $E_s$  is the unit  $2 \times 2$  matrix. The matrix function  $\chi_1^{\nu}$  can be found from (3.14).

Now we discuss the choice of the model potential. We will consider a tube with soft walls and with the same elliptic cross-section [81], which can be modeled by using the potential

$$v_{\text{int}}(x, y) = v_{\text{int}}\left(x^*, \frac{\Phi(x)^{-1}\mathbf{y}}{D(x)}\right), \quad v_{\text{int}}(x^*, y) = \left[ \left(\frac{y_1}{a}\right)^2 + \left(\frac{y_2}{b}\right)^2 \right]^m, \quad m > 0. \quad (4.41)$$

Passing from the variables  $y = (y_1, y_2)$  to the new variables  $y' = (y'_1, y'_2)$  determined by the relation  $y = D^{\nu} y'$ ,  $\gamma = m/(m+1)$ , we obtain  $\varepsilon_{\perp}^{\nu}(x) = D(x)^{-2\gamma} \varepsilon_{\perp}^{\nu}(0)$ . It is easy to see that the dispersion  $d(x)$  with respect to the coordinates  $y$  in the state  $w_n^{\nu}$  depends on  $x$  according to the relation  $d(x) = D(x)^{-\gamma} d(0)$ . It is natural to assume that  $d(x)$  is *proportional* to the linear dimensions of the tube section. Then  $D^{\nu}$  is the “soft” coefficient of extension of the section, and  $\gamma$  is the stiffness coefficient of the walls. The dependence of the energy on  $x$  can be represented as

$$\varepsilon_{\perp}^{\nu}(x) = \varepsilon_{\perp}^{\nu}(0) \frac{d(0)^2}{d(x)^2}. \quad (4.42)$$

As  $m \rightarrow \infty$ , the potential (4.41) disappears in the interior of the domain and tends to  $\infty$  outside this domain; the coefficient  $\gamma \rightarrow 1$  and  $d(x) \rightarrow D(x)^{-1} d(0)$ . In the limit, we obtain the “empty cylinder” model:  $v_{\text{int}}(x^*, y) = 0$  for  $(y_1/a)^2 + (y_2/b)^2 \leq 1$  and  $v_{\text{int}}(x^*, y) = \infty$  for  $(y_1/a)^2 + (y_2/b)^2 > 1$ , where  $D(x)$  is the coefficient of extension (of homothety). As in the case of nanofilms, we introduce additional “rigid” walls in the area where the wave function is exponentially small.

Taking into account the form of potential (4.41), we obtain the relation

$$w_j^{\nu}(x, y) = \frac{1}{D(x)} w_j^{\nu}\left(x^*, \frac{\Phi(x)^{-1}\mathbf{y}}{D(x)}\right), \quad j = 1, \dots, r. \quad (4.43)$$

#### 4.6.6. Remark

Calculating  $\chi_0^{\nu}$ , we do not fix any special form of the functions  $w_1^{\nu}, \dots, w_r^{\nu}$ . We assume that they form an orthonormal basis in the eigenspace of problem (4.38) corresponding to the eigenvalue (term)  $\varepsilon_{\perp}^{\nu}(x)$  with the number  $\nu$  and depend smoothly on all its variables. Of course, such a basis is not unique, and it is convenient to make its final choice in the subsequent construction of asymptotic solutions. For example, sometimes  $w_j^{\nu}$  can be taken to be the eigenfunctions of the momentum operator  $\hat{l}$ , i.e., in this case, it is necessary to distinguish the states inside the term according to the projections of the orbital momentum in these states

on the tube axis. Then the momentum matrix  $\Lambda$  is diagonal. Of course, it is also possible to change the basis in the space of spinors; this is convenient for the case in which the spin affects the classical dynamics (see below the “medium-wave regime”). Obviously, the choice of a new basis is equivalent to the inclusion of some unitary  $2r \times 2r$  matrix depending on  $x$  into formula (4.37) after the operator  $\hat{\chi}^\nu$ .

#### 4.6.7. Effective Hamiltonians of longitudinal motion

Using formulas from Section 3, we obtain  $L_0^\nu$  and  $L_1^\nu$ . In general, the objects  $\Lambda$ ,  $L_y$ , etc. introduced below also depend on the number  $\nu$  (as well as  $\chi_j$ ,  $L_j^\nu$ , and  $\psi^\nu$ ). Sometimes, we omit this dependence to simplify the notation.

The symbols  $L_0^\nu$  and  $L_1^\nu$  are determined as follows:

$$\begin{aligned} L_0^\nu(p, x) &= H_{\text{eff}} E_r \otimes E_s, \\ L_1^\nu(p, x) &= ik/2(\mathbf{n}, \mathbf{A}_0) E_r \otimes E_s + L_y \otimes E_s + E_r \otimes L_s + L_{sy}, \quad L_s = -\frac{1}{2}\langle \boldsymbol{\sigma}, \mathbf{H} \rangle, \\ L_y(p, x) &= \left( (\partial_x \Phi) p - 1/2 \langle \partial_x \mathbf{R}, \mathbf{H} \rangle \right) \Lambda - \langle \mathbf{Y}_\perp, \mathbf{H} \rangle p + \left\langle \mathbf{Y}, \nabla v_{\text{ext}} + \frac{\partial \mathbf{A}_0}{\partial t} + kp^2 \mathbf{n} \right\rangle, \\ L_{sy}(p, x) &= \mu^{-1} \alpha \left( M^0 \otimes \langle \boldsymbol{\sigma}, \partial_x \mathbf{R} \rangle + M^1 \otimes \langle \boldsymbol{\sigma}, \mathbf{n}_1 \rangle + M^2 \otimes \langle \boldsymbol{\sigma}, \mathbf{n}_2 \rangle \right). \end{aligned} \quad (4.44)$$

By  $E_r$  we denote the unit  $r \times r$  matrix, by  $\Lambda(x)$  we denote the  $r \times r$  momentum matrix with elements  $\Lambda_{jj'} = \left\langle w_j^\nu, \hat{L} w_{j'}^\nu \right\rangle_y$ , by  $M^j(x)$  we denote the  $r \times r$  matrix of the form  $(M^0)_{jj'} = -i \left\langle w_j^\nu, ((\partial_1 v_{\text{int}}) \partial_2 - (\partial_2 v_{\text{int}}) \partial_1) w_{j'}^\nu \right\rangle_y$ ,  $(M^1)_{jj'} = \left\langle w_j^\nu, (\partial_2 v_{\text{int}}) w_{j'}^\nu \right\rangle_y$ ,  $(M^2)_{jj'} = -\left\langle w_j^\nu, (\partial_1 v_{\text{int}}) w_{j'}^\nu \right\rangle_y$ , where  $\partial_i = \partial / \partial y_i$ , and by  $\mathbf{Y}(x) = Y_1 \mathbf{n}_1 + Y_2 \mathbf{n}_2$ ,  $\mathbf{Y}_\perp(x) = Y_2 \mathbf{n}_1 - Y_1 \mathbf{n}_2$  we denote the three-dimensional “vectors” whose components are the  $2 \times 2$  “dipole” matrices  $(Y_i)_{jj'}(x) = \left\langle w_j^\nu, y_i w_{j'}^\nu \right\rangle_y$ ,  $i = 1, 2$ . As above,  $\langle \cdot, \cdot \rangle_y$  denotes integration over the variables  $y$ . The symbol  $L_2^\nu(p, x)$  is significantly more complicated, but we need only a part of it, *viz*, the so-called “geometric potential”  $\mathcal{G}(x) = -(k^2(x)/8) E_r \otimes E_s$ . In the long-wave approximation, it is necessary to take this term into account. It is precisely this term that generates bound states in an empty waveguide [55].

#### 4.6.8. Additional boundary and initial conditions

Formulas (4.44) allow one to construct the leading term of different asymptotic solutions to the effective equation of adiabatic (longitudinal) motion of the  $\nu$ th subband of a dimensional quantization. To perform more complete constructions, one has to sum solutions with different values of  $\nu$ . But from a physical point of view, one is interested in the *reduced equations with only small  $\nu$* , and it usually suffices to consider the case of several  $\nu$ . (In nanotubes,  $\nu$ , as a rule, does not exceed 7 [64]). This fact turns out to be very important later in the study of equations in curved waveguides and tubes and allows one to ignore the applicability problem for the asymptotic formulas obtained for large  $\nu$ , and the convergence problem for the corresponding series with respect to  $\nu$ . For this reason, *it suffices to pose the additional boundary and initial conditions already not for the original equation, but for finite (here one-dimensional) (simplified) equations of the form (3.7)*. Using the physical terminology, we can say that it is of interest to study the longitudinal dynamics of a small set of subregions of transverse quantization. The corresponding additional conditions for the case of spatial waveguides will be posed accurately below.

## 5. Asymptotic solutions to the effective equations of adiabatic motion

Now we want to discuss the question about solutions to the reduced effective equations of adiabatic motion. The existence of the *adiabatic* parameter  $\mu$  allows one to separate the *fast motion* from the *adiabatic motion* (the electron motion from the nuclei motion in a molecule, the transverse motion from the longitudinal motion in a waveguide, electron waves from the lattice oscillations in crystals, etc.). A very important fact is that the parameter  $\mu$  slightly depends on the energy of the adiabatic motion in a certain range where it varies. The fact that the adiabatic approximation holds for the entire region of energies of adiabatic motion is well known in physical literature (see, *e.g.*, [82]). The adiabatic motion can be essentially different for different energies from this region. This fact is important if one is interested in the construction of asymptotic or exact solutions to the reduced equation of adiabatic motion describing different physical processes (and corresponding to different energies). This means that asymptotic and sometimes exact solutions are of different type and thus the process of determining the leading (or essential) part of the symbol  $L$  should be revised. For instance, some parts of the correction  $L_1$  must be moved to the leading part of  $L$ . As we also mentioned, this fact can, in turn, change the definition of the characteristics of the reduced equation and, in particular, lead to the “semiclassical splitting” of terms in the degenerate case (when  $r \neq 1$ ). In the case of nanotubes, this effect shows how the spin affects the determination of classical characteristics. We think that the best way to explain these phenomena is to consider a simple nontrivial example which, in our opinion, is the problem of quantum waves in nanotubes. Thus, we restrict ourselves to this example bearing in mind its importance. Moreover, it seems advisable to explain the main ideas and considerations with the example of the Schrödinger equation with the Hamiltonian

$$\hat{\mathcal{H}} = -\frac{\mu^2}{2} \Delta_x - \frac{1}{2} \Delta_y + v(x, y), \quad (5.1)$$

where  $x \in \mathbb{R}^n$  and  $y \in \mathbb{R}^k$ . This will be done in Section 5.1. If one chooses an appropriate potential  $v(x, y)$ , this equation describes problems of molecular physics, as well as of quantum waveguides. The ideas from Section 5.1 are applied to the problem of quantum waves in nanotubes in Section 5.2.

As we mentioned above, the semiclassical analysis of the reduced effective equation for adiabatic motion is well developed and the solutions for the above-listed problems are given in the simplest form by using the Maslov canonical operator [6, 83]. To obtain explicit formulas is a task which must be tackled in concrete situations. There are many publications devoted to the Maslov canonical operator. Here we only note that this is actually a certain algorithm whose realization, as well as the process of obtaining an answer appropriate from an applications point of view (*e.g.*, solution plots, calculation of scattering data, beating frequency, etc.), even in the one-dimensional situation, requires additional effort and the use of computers. A detailed description of the solutions based on this algorithm and concrete physical results are outside the scope of this work. Such results are the focus of other publications (see, *e.g.*, [84, 85]). Here, in Section 5.3, we will only very briefly describe the asymptotic solutions and the simplest physical results. This remark also concerns all the examples considered in this paper.

The majority of the ideas stated below in Section 5.1 can be generalized to other examples that were discussed above. Nevertheless, it is necessary to emphasize that a “simple” Hamiltonian of the form (5.1) has a very special form, and hence some effects related to this Hamiltonian do not occur in examples with other Hamiltonians. On the other hand, if the Hamiltonian has a different form, then other interesting effects may appear.

## 5.1. GENERAL CONSIDERATIONS

5.1.1. *Internal and external parameters*

In the examples under study, we implicitly assume that the dimensionless coefficients (e.g., the potential  $v_{\text{ext}}$  in nanofilms and nanotubes) is independent of  $\mu$ . Indeed, in real situations, it is sometimes natural to assume that the coefficients can depend on both  $\mu$  and other parameters. These parameters characterize the kinetic energy of adiabatic motion, the strength of external fields, the strength of interactions, etc. In this case, the functions  $\chi_0^\nu, \chi_1^\nu, \dots, L_0^\nu, L_1^\nu, \dots$  in formula (3.9) also depend on these parameters. Nevertheless, under appropriate constraints, the formula for the separation of variables (3.9) remains valid. For purposes of mathematical rigor, some constraints must be imposed on these problem parameters so as to connect them, for example, with the parameter  $\mu$ . However, in this case, one must bear in mind that, in concrete situations, all these parameters are numbers, and such constraint formulas are of a very conventional character. For this reason, to avoid cumbersome notation, we present the explicit dependence on such parameters only when necessary.

5.1.2. *Semiclassical parameter  $h$* 

The fact that the solutions of the equation of adiabatic motion can be essentially different originates from the existence of an additional parameter, which characterizes the excitations of the adiabatic subsystem in the allowable range. To introduce this parameter, we consider the first well-known asymptotics of Equation (2.5) corresponding to different energies in the case of the Hamiltonian  $\hat{\mathcal{H}}_0 = \frac{1}{2}(-i\mu \frac{\partial}{\partial x})^2 + \frac{1}{2}(-i \frac{\partial}{\partial y})^2 + v(x, y)$ . Denote, for the moment, by  $\langle \cdot, \cdot \rangle$  the inner product in the original configuration space. The kinetic energies of fast and adiabatic motions in this situation are  $\mathbf{K}_f = \langle \Psi, \frac{1}{2}(-i \frac{\partial}{\partial y})^2 \Psi \rangle$  and  $\mathbf{K}_a = \langle \Psi, \frac{1}{2}(-i\mu \frac{\partial}{\partial x})^2 \Psi \rangle$ , respectively.

As we mentioned above, according to [6], the semiclassical solutions to Equation (3.7) have the WKB-form  $\Psi \approx \chi(\partial S/\partial x, x, y)\psi(x, t, \mu)$ ,  $\psi \approx \exp(iS(x, t)/\mu)\varphi(x, t, \mu)$ , where the function  $\varphi(x, t, \mu)$  depends regularly on  $\mu$ . In this case, the kinetic energies of fast and adiabatic motions have the *same order*:  $\mathbf{K}_f \sim \mathbf{K}_a \sim 1$ . This solution corresponds to the *excited state* of adiabatic motion. On the other hand, Born and Oppenheimer [1, 3] constructed the harmonic-oscillator-type solution  $\Psi \approx \chi(x, y, \mu)\psi(x, \mu)$ ,  $\psi \approx \exp(-x^2/\mu)$ . This solution corresponds to the kinetic energy  $\mathbf{K}_a \sim \mu$ ; hence the energy of adiabatic (nuclei) motion in this case is much smaller than the energy of fast motion. Further, in the theory of waveguides, we sometimes have solutions of the form  $\Psi \approx \chi(y, x, \mu)\psi(x, t, \mu)$ , where  $\chi(y, x, \mu)$ ,  $\psi(x, t, \mu)$  depend regularly on  $\mu$ . For these solutions, we obtain  $\mathbf{K}_a \sim \mu^2$ . The above-listed different asymptotics can be classified by the parameter  $h = \mu\sqrt{\mathbf{K}_f/\mathbf{K}_a} \Leftrightarrow \mathbf{K}_a/\mathbf{K}_f \sim \mu^2/h^2$ . We call  $h$  the *semiclassical* parameter. Let us emphasize that the adiabatic parameter is always assumed to be small and, conversely, the parameter  $h$  can be small but also  $\sim 1$ .

This parameter can be explained in another way. For clarity, we consider the plain straight quantum waveguide and, for a while, return to dimensional variables. We have the diameter  $d_0$  and the length  $l_0$  of the waveguide. Recall that our goal is to construct asymptotic solutions of the reduced equation which describe the motion along the tube axis in a sufficiently wide range of longitudinal energies and the transverse wavelength  $\lambda_\perp \sim d_0$ . To the longitudinal energy, there corresponds the characteristic de Broglie wavelength  $\lambda_\parallel = \hbar/p_\parallel$ , where  $p_\parallel$  is the dimensional momentum of longitudinal motion. Now the “*semiclassical*” parameter is  $h = \lambda_\parallel/l_0$ . In other words, the parameter  $h$  determines the “smoothness” of the function  $\psi$  ( $h^{-1}$  is the number of oscillations at the distance  $\sim l_0$ ) and agrees with the estimation of its derivatives:  $\langle \psi, \frac{\partial \psi}{\partial x} \rangle \sim h^{-1}$ .



We again consider the example of an empty waveguide. Then the energy of the longitudinal motion on the  $\nu$ -th subband of transversal quantization has the form:  $p_{\parallel}^2/2m + v_{\text{eff}}(x)$ , where  $v_{\text{eff}}(x) = v_{\text{ext}}(x) + v^2\pi^2\varepsilon_{\perp}$ ,  $\varepsilon_{\perp} = \hbar^2/(2md_0^2)$ . Denote by  $p_{\perp}$  the transverse momentum. Taking into account the relation between the de Broglie wavelength and the corresponding momentum, we obtain  $\frac{p_{\parallel}}{p_{\perp}} \sim \frac{\hbar/\lambda_{\parallel}}{\hbar/\lambda_{\perp}} \sim \frac{d/l_0}{\lambda_{\parallel}/l_0} \sim \frac{\mu}{\hbar}$ . Thus, the kinetic energies of longitudinal (adiabatic) and transverse (fast) motions satisfy the relations  $\mathbf{K}_{\mathbf{a}}/\mathbf{K}_{\mathbf{f}} \sim \mu^2/h^2$  and  $\mathbf{K}_{\mathbf{f}} \sim \varepsilon_{\perp}$ . Now we return to dimensionless variables. Then the dimensionless longitudinal kinetic energy is  $\mathbf{K}_{\mathbf{a}} = p_{\parallel}^2/2 \sim \mu^2/h^2$ . It is clear that, if a particle moves along the waveguide, then the kinetic energy can vary under the action of the force  $f = -\partial v_{\text{eff}}/\partial x$ . For this force  $f$  not to accelerate the particle so that its kinetic energy be of an order different from  $\mu^2/h^2$ , it is necessary that its work does not exceed, in the order of magnitude, the parameter of the characteristic kinetic energy corresponding to the initial momentum. In dimensionless variables, to the distance  $\sim l_0$  there corresponds an interval  $\sim 1$ . Hence the work of the force  $f$  is of the order of the derivative  $\partial v_{\text{eff}}/\partial x$ . This implies that the effective potential must have the form  $v_{\text{eff}} = v_{\text{eff}}^0 + \frac{\mu^2}{h^2} v_{\text{eff}}^1(x)$ , where  $v_{\text{eff}}^0 = \text{const}$  and  $v_{\text{eff}}^1(x)$  can, in general, regularly depend on the parameters  $\mu$  and  $h$ . Moreover, the work can be even equal to zero, since the characteristic longitudinal momentum is determined not only by the variable part  $v_{\text{eff}}^1(x)$  of the effective potential, but also by the “input” momentum of the wave packet under study (*i.e.*, by the gradient of the phase of the wave function at the initial time instant in the Cauchy problem or by the momentum of the incident wave in the scattering problem). In the last case, the asymptotics of the wave function can be obtained by using the well-known Born approximation.

*Remark*

We point out that  $v_{\text{eff}}$  is determined by both the external field and the field of the crystal. Therefore in the case of a quantum waveguide, the above constraints lead, in particular, to the assumption that the geometric parameters of the waveguide, *i.e.*, the curvature (and torsion) of its axis, the width, etc., vary sufficiently “slowly.”

5.1.3. *Characteristic time scale and the reduced equation consistent with this scale*

The question concerning the time scaling is nontrivial and, generally speaking, can be resolved separately in each concrete problem. It is natural to understand what characteristic time is required for a quantum particle to traverse a certain characteristic distance. For problems in nanotubes, the characteristic distance is the total tube length (*e.g.*, in the scattering problem or in the problem of the wavetrain propagation) or the size of the “localization area” of the wave function in the problem of bound states. For the moment, we assume the characteristic distance to be of the order of  $l_0$  in dimensional variables or to be  $\sim 1$  in dimensionless variables. One has to replace the time scaling by the energy scaling in the case of stationary problems (for instance, in problems of electron-phonon interaction or in molecular physics).

*Remark*

To introduce the characteristic time scale in the general case, we can use the following ideas. It is clear that the characteristic time scale is  $t \sim a/\langle v \rangle$ , where  $a$  is the characteristic distance for adiabatic motion and  $\langle v \rangle$  is the mean velocity. Generally speaking,  $a$  as well as  $\langle v \rangle$  depend on the “longitudinal” kinetic energy. In quantum mechanics, we have  $\langle v \rangle = d\langle x \rangle/dt$ . Using (2.2), we obtain  $d\langle x \rangle/dt \sim i\mu^{-1} \langle [\hat{p}^2/2, x] \rangle = \langle \hat{p} \rangle = \mu/h$  (*cf.* Section 3.3.3). Thus we have  $t \sim (h/\mu)a$ . For the scattering problem, the wavetrain-propagation problem and some other

problems, we can set  $a \sim 1$ . For lower-bound states and trapped modes we have to set  $a \sim h \sim \sqrt{((\Delta x)^2)}$ .

The dimensionless time  $t$  used in the general scheme for Equation (2.2) was actually chosen for the case  $p_{\perp} \sim p_{\parallel}$ , *i.e.*, for the case  $\mu/h \sim 1$ . If this relation does not hold, the time of passage of a particle through the waveguide, which is naturally understood as the characteristic time of the problem, must be multiplied by the factor  $(h/\mu)$ . Therefore, instead of  $t$ , it is convenient to introduce a new dimensionless time  $t'$  by the relation  $t = (h/\mu)t'$ .

In the case of nanotubes this redefining of the time scale becomes consistent with the preceding physical argument because of the following transformations in (3.7). The term  $v_{\text{eff}}^0$  results only in a displacement (renormalization) of the energy in the stationary problem generated by the reduced equation; or the factor  $\exp(-iv_{\text{eff}}^0 t'/\mu)$  appears in the wave function  $\psi^v$  of the nonstationary Schrödinger equation (3.7). Taking this into account, we represent the solution of this equation in the form  $\psi^v = \exp(-iv_{\text{eff}}^0 t'/\mu) \psi'^v$ , where  $\psi'^v(x, t)$  is a new unknown function. Since we assume that  $p \sim \mu/h$ , it is natural to divide the equation by the parameter  $\mu^2/h^2$ . In the left-hand side this gives the derivatives  $i(h^2/\mu) \frac{\partial \psi'^v}{\partial t'}$ , which, after the above change of time, take the form  $i h \frac{\partial \psi'^v}{\partial t'}$ . It is important to point out that this transformation concerns only the time variable: the variables  $x$  and  $y$  are not transformed. As a result, instead of (3.7) and (4.44) taking the corrections  $L_1^v$ ,  $L_2^v$ , etc., into account, we obtain the equation (the primes are omitted):

$$i h \frac{\partial \psi^v}{\partial t} = \left\{ \frac{1}{2} \left( -i h \frac{\partial}{\partial x} \right)^2 + v_{\text{eff}}^1 + \frac{h^2}{\mu} \left[ L_1^v \left( \frac{\mu}{h} \left( -i h \frac{\partial}{\partial x} \right), \hat{x} \right) + \mu L_2^v \left( \frac{\mu}{h} \left( -i h \frac{\partial}{\partial x} \right), \hat{x} \right) + \dots \right] \right\} \psi^v. \quad (5.2)$$

#### 5.1.4. Accuracy of asymptotic expansions

The number of terms in the expansion of the intertwining operator  $\hat{\chi}$  and the operator  $\hat{L}$  can be arbitrarily large. However, as we already mentioned, to calculate terms of these series explicitly, even lower-order ones, is, as a rule, a very complicated problem. Therefore, it is natural to consider only the terms for which one can correctly estimate the *leading term* of the asymptotics of the wave function or of the energy value. It is reasonable that the notion of the “leading” term of an asymptotics can be determined not only by the adiabatic parameter  $\mu$ , but also by the “semiclassical parameter”  $h$ , which is related to the form of the coefficients and the solution of the effective equation of adiabatic motion. We shall return to the question about numbers of terms in the intertwining operator  $\hat{\chi}$  and the operator  $\hat{L}$  later. Now we recall well-known estimates which allow us to estimate these numbers.

Taking in account this fact, let us discuss the problem of choosing the number of terms in the expansion of the symbols of the operator  $\hat{L}$  and the intertwining operator  $\hat{\chi}$ . Again, we restrict our consideration to the case of nanotubes, although the main ideas can be generalized for the majority of the adiabatic problems listed above, including the non-self-adjoint problems like water waves in a pycnocline (problems of such type usually appear in hydrodynamics).

Since the problem contains two parameters  $\mu$  and  $h$ , we shall calculate as many terms as we need to construct the leading term of the asymptotics with respect to  $\max(h, \mu)$  if  $h \ll 1$  and with respect to  $\mu$  if  $h = 1$ . (Recall that the parameter  $\mu$  is always assumed to be small, and the parameter  $h$  can be either small or of order  $O(1)$ .) To find the minimal reasonable number of terms in an asymptotic expansion, it is natural to use the well-known estimate for the solution of the Cauchy problem for a nonhomogeneous Schrödinger-type equation:  $i\varepsilon \frac{\partial \phi}{\partial t} =$

$\hat{A}\phi + f$ ,  $\phi|_{t=0}=0$ . Here  $\hat{A}(t)$  is an essentially self-adjoint (for each  $t$ ) operator in  $L_2$ , and  $\varepsilon > 0$ . Let  $\phi$  be a solution of this problem; then the following inequality holds for any  $t$  from the fixed interval  $[0, T]$ :  $\|\phi\|_{L_2} \leq \frac{T}{\varepsilon} \max_{t \in [0, T]} \|f\|_{L_2}$ .

We assume that  $\psi_{\text{ex}}$  is an exact solution of the original equation (3.7) and  $\Psi_{\text{as}}$  is its asymptotic solution of the form (3.9) and these solutions coincide at the zero time instant; moreover,  $\psi_{\text{as}}$  satisfies the original equation with discrepancy  $f_{\text{as}}$ . For the operator  $\hat{A}$ , we choose the original quantum Hamiltonian and set  $\varepsilon = \mu$  and  $T = \frac{h}{\mu} T_0$ , where  $T_0$  is independent of  $h$  and  $\mu$ . Then we obtain the estimate

$$\|\psi_{\text{as}} - \psi_{\text{ex}}\| \leq \frac{h}{\mu^2} T_0 \max \|f_{\text{as}}\|_{L_2} \quad (5.3)$$

for the difference  $\phi = \psi_{\text{as}} - \psi_{\text{ex}}$ . This implies that the minimal reasonable number of terms in the expansion of the symbols of the operators  $\hat{\chi}$  and  $\hat{L}$  in formulas (3.6) and (3.8) must at least satisfy the condition  $\frac{h}{\mu^2} \|f_{\text{as}}\|_{L_2} \ll 1$  for  $\mu \ll 1$ . Of course, it should be remembered that the norm of the discrepancy  $f_{\text{as}}$  depends on  $\mu$  and  $h$ . As a heuristic argument, it is also useful to apply the estimate (5.3) to the reduced Equation (3.7).

### 5.1.5. Classification of quantum states for longitudinal motion

We return to the passage from (3.7) to (5.2). For  $h \ll 1$ , to construct a wave function, it is natural to use the semiclassical approximation. Outside a neighborhood of the focal points (the turning points), the typical asymptotics of a wave function with characteristic wavelength  $\lambda_{\parallel} \sim h$  is given by the WKB-solution

$$\psi(x, t) = A(x, t, h) \exp\left(\frac{iS(x, t)}{h}\right), \quad A(x, t, h) = A(x, t, 0) + O(h), \quad (5.4)$$

where  $S(x, t)$  is the phase and  $A(x, t, h)$  is, in general, the vector amplitude. As is known [6], in the first approximation, after the substitution of this function into the original equation, the operator  $-i\hbar \frac{\partial}{\partial x}$  is, in the leading part, replaced by  $\frac{\partial S}{\partial x}$ , and thus the order of the terms

in the operators  $h^2 \mu^{j-2} L_j^{\nu}(\bar{x}, \frac{\mu}{h}(-i\hbar \frac{\partial}{\partial x}))$  in (5.2) is determined by the order of the functions  $L_j^{\nu}(x, \frac{\mu}{h} \frac{\partial S}{\partial x})$ . This fact leads to the well-known conclusion that the phase  $S(x, t)$  is determined by the classical Hamiltonian system whose Hamiltonian is the leading part of the symbol expansion with respect to the parameter  $h$ . Bearing this in mind, it is natural to define the operator  $\hat{p}^h = -i\hbar \partial / \partial x$ , rather than the operator  $\hat{p} = -i\mu \partial / \partial x$ , to be the momentum operator. Clearly, for  $\mu = h$ , the classical Hamiltonian is the effective Hamiltonian (3.13), but if the adiabatic and semiclassical parameters  $\mu$  and  $h$  are of different orders and  $h \ll 1$ , then to construct a semiclassical asymptotic scheme it is necessary to write the expansion with respect to parameter  $h$ , assigning  $\mu = \mu(h)$ . As we shall see later, in some cases, additional terms from  $L_1^{\nu}$  will be included in the classical Hamiltonian (subject to the expansion with respect to  $h$ ).

Now let us discuss how many terms in the expansion of the operator in the right-hand side of (5.2) we must have to find the leading part of its asymptotic solution. By setting  $\varepsilon = h$  and applying the estimate (5.3) to Equation (5.2), we see that, at least intuitively, it suffices to calculate the effective Hamiltonian  $(p^h)^2/2 + v_{\text{eff}}^1$  and the first correction  $L_1^{\nu}(x, \frac{\mu}{h} p^h)$ . This conclusion is consistent with the well-known fact from the theory of semiclassical asymptotics: terms of the order of  $h^2$  (and even of  $h^{1+\delta}$ ,  $\delta > 0$ ) do not affect the phase  $S(x, t)$  and the leading part of the amplitude  $A(x, t, 0)$ . This conclusion has a general character and holds always if it is assumed that  $\mu \leq h \ll 1$ , i.e., for the case in which the semiclassical approximation can be used. At the same time, as we just noted, concrete formulas can essentially differ

in the following situations: (a) if  $\mu$  and  $h$  have the same order ( $\mu \sim h$ ) and (b) if  $\mu \ll h$ . If the parameter  $h \sim 1$ , then the semiclassical approximation cannot be used, but Eq. (5.2) remains to hold and can even be simplified, although in this case a part of  $L_2^v$  must be taken into account. The existence of these differences results in the following classification of asymptotic solutions depending on the relation between the parameters  $\mu$  and  $h$  (or, which is equivalent, depending on the relation between the longitudinal  $\mathbf{K}_a$  and transverse  $\mathbf{K}_f$  kinetic energies in the waveguide).

(a) For  $h = \mu$ , we have the standard “semiclassical” situation [6] or the “short-wave” regime in which the “longitudinal” energy is of the same order as the energy of transverse motion and  $d \sim \lambda_{\parallel} \ll l_0$  in dimensional variables. Then the effective adiabatic and semiclassical Hamiltonians, as well as the corrections to them, coincide, and to find the leading term of the asymptotics of the wave function, the complete description of the effective Hamiltonian and the first correction is required.

(b) In this case, which is naturally called the “medium-wave” regime,  $\mu \ll h \ll 1$ , the “longitudinal” energy of the mode is significantly less than that of the “transverse” mode and  $d < \lambda_{\parallel} \leq \sqrt{l_0 d}$  in dimensional variables. Then, expanding the correction  $L_1^v$  with respect to the parameter  $\mu/h$ , for the symbol of the operator, we obtain

$$L^v = \left( \frac{(p^h)^2}{2} + v_{\text{eff}}^1 + \frac{h^2}{\mu} L_1^v(x, 0) \right) + h \frac{\partial L_1^v}{\partial p}(x, 0) p^h + h \cdot O\left(\frac{\mu}{h}\right).$$

This implies that the nondifferential part  $\frac{h^2}{\mu} L_1^v(x, 0)$  of the first adiabatic correction in the expansion of the operator  $\hat{L}_1^v$  can be transferred into the semiclassical effective Hamiltonian. This is clearly seen in the case  $h = \sqrt{\mu}$ . Then the semiclassical effective Hamiltonian becomes equal to  $\frac{(p^h)^2}{2} + v_{\text{eff}}^1 + L_1^v(x, 0)$ . Moreover, for  $h^2 \gg \mu$ , the term  $\frac{h^2}{\mu} L_1^v(x, 0)$  can play a determining role. Then an argument similar to that in Section 2.6 shows that this term “accelerates” the particle in the longitudinal direction so that the characteristic longitudinal momentum in dimensionless variables takes the value  $\sqrt{\mu}$ . In other words, in this case, for the parameter  $h$  we must take the parameter  $\sqrt{\mu}$ , and we return to the situation considered above, but with  $v_{\text{eff}}^1$  multiplied by a small value. Clearly, if  $L_1^v(x, 0) = 0$ , the above argument is meaningless. But, as we shall see later, such a term appears in nanotubes both due to their geometry and due to the external electromagnetic field. In this case, there arise some additional parameters, e.g., field amplitudes, and these parameters can effectively decrease the value of  $L_1^v(x, 0)$  and thus compensate the increase caused by the parameter  $h^2/\mu$ . We also note that the terms in the operator  $\hat{L}_1^v$  containing the second- and higher-order derivatives (corresponding to higher powers in the expansion of  $L_1^v$  with respect to the variable  $p^h$ ) can be omitted in the calculations of the leading term of the semiclassical asymptotic solution, although, of course, these terms do not decrease the accuracy.

#### *Remark*

If the main part of the Hamiltonian is quadratic with respect to the momenta, the Hamiltonian preserves its form. In the other examples considered above (e.g., for equations with rapidly oscillating coefficients, for waves in picnocline), the leading part of the adiabatic Hamiltonian  $L_0$  depends on the momentum  $p$ . Therefore, this expansion changes the structure of the leading part. For example, in the problem with rapidly oscillating coefficients (electron waves in crystals),  $L_0$  is replaced by its expansion with respect to  $p$  in a more complex way (non-quadratically). Moreover, this expansion, as a rule, begins with terms that are

quadratic with respect to  $p$ . The coefficient before  $p^2$  is inversely proportional to the *effective mass* (see [4]).

(c) If the parameter  $h \sim 1$ , the semiclassical approximation cannot be used, and the wave functions oscillate, if at all, rather slowly and in the dimensional variables  $\lambda_{\parallel} \sim l_0$ . According to the above, this situation is possible only if  $L_1^{\nu}(x, 0) \equiv 0$ . But the adiabatic approximation works, and from (5.2) one can easily derive the equation for the leading term of the asymptotics of the (smooth) wave function  $\psi(x, t)$  on the waveguide axis. For this, it suffices to set  $h = 1$  in (5.2) and then to let  $\mu \rightarrow 0$ . As a result of this passage to the limit, which is naturally called the *long-wave approximation*, we obtain the equation

$$i \frac{\partial \psi}{\partial t} = \left[ \frac{1}{2} \frac{\partial^2}{\partial x^2} + v_{\text{eff}}^1 - i \frac{\partial L_1^{\nu}}{\partial p}(x, 0) \frac{\partial}{\partial x} + L_2^{\nu}(x, 0) \right] \psi.$$

*Remark*

As already noted for the Helmholtz operator in plane one-mode waveguides, such an equation was first obtained in [55], where, in particular, it was proved that one can organize a single bound state in the waveguide by choosing an appropriate curvature of the waveguide. An equation similar to (5.11) and several consequences of it were obtained in [31–36, 57, 58]. We also note that equations of this type are close to the equations obtained as the result of averaging or homogenization in the theory of wave processes in media with rapidly varying characteristics [40, 86–88].

(d) Finally, we can consider the case in which  $\mu \gg h$  or, in dimensional variables,  $\lambda_{\parallel} \ll \lambda_{\perp} \ll l_0$ . This case is naturally called the “ultrashort-wave” regime. For Equation (5.2) to be meaningful, it is necessary to impose additional constraints on the behavior of the functions  $L_j^{\nu}$  in the variable  $p$ . We consider only the case for which  $L_j^{\nu}$  are polynomials of a degree not exceeding 2 with respect to  $p$ . Then it is easy to show that the semiclassical approximation for any  $\mu \gg h$  can be applied to Equation (5.2). However, this is not sufficient for reconstructing the asymptotic solution of the original Schrödinger equation in the waveguide from the function  $\psi(x, t)$  by formula (3.9). For example, if the first correction  $\chi_1^{\nu}$  in the expansion of the symbol of the intertwining operator  $\hat{\chi}^{\nu}$  in formula (3.6) depends linearly on  $p$ ,  $\mu \geq h^2$ , and a rapidly oscillating function of the form (5.4) is taken to be  $\psi$ , then the function  $\mu \hat{\chi}_1 \psi$  turns out not to be small. In this sense, the expansion of the operator  $\hat{\chi}$  in powers of  $\mu$  is not an asymptotic expansion. For this reason, as we shall see below, the ultrashort-wave approximation for curved nanotubes can be used for the case in which  $h^2 \ll \mu \ll h$ . We can also note that, in the ultrashort-wave case, the actual effective potential  $v_{\text{eff}}^1$  is small so that it can be transferred into  $L_1^{\nu}$  or even completely omitted. Then the semiclassical effective Hamiltonian coincides with the Hamiltonian of a free particle, and hence, in this case, the semiclassics is simply the Born approximation.

*Remark*

It should be remembered that, in actual calculations, the above classification (in the parameters  $\mu$  and  $h$ ) must be made more precise, which concerns the values of both the external fields and the crystal field, as well as the relations between them. Of course, in this case, the corrections can also be included into the leading part of the symbol (in the classical Hamiltonian), which, however, can unnecessarily complicate the procedure for constructing the asymptotic solutions. On the other hand, as already noted, in a real situation, each parameter is a concrete small number, and hence the further detailing of how the effective Hamiltonian and corrections to it depend on the relation between the parameters  $\mu$  and  $h$  has an academic,

rather than practical, character. Taking this consideration into account, it is convenient, from a mathematical point of view, to fix the relations between the parameters  $\mu$  and  $h$ , assuming for the respective regimes that (a),  $h = \mu$ , (b),  $h = \sqrt{\mu}$ , (c),  $h = 1$ , (d),  $h = \mu^{3/2}$  and including the “remaining” parts of the relations between  $\mu$  and  $h$  into the coefficients of the equation (such as the strengths of electric and magnetic fields, curvature, etc.).

The suggested classification can be used in the general situation. But in certain cases some regimes (like the ultrashort-wave region or the long-wave region) do not exist. Anyway the question of the existence of solutions for a certain fixed  $h$  should be solved individually.

### 5.1.6. *The number of terms in the intertwining operator*

We assume that we use the dimensionless time  $t$  consistent with the semiclassical parameter  $h$  (see Subsection 5.1.3). Suppose that we have kept  $N$  terms in the expansion of the symbols of the operators  $\hat{\chi}^\nu$  and  $\hat{L}^\nu$  determined by the coefficients  $\chi_j^\nu$  and  $L_j^\nu$ . Suppose also that we have constructed a function  $\psi^\nu$  satisfying the reduced Equation (5.2) with accuracy up to a discrepancy  $f$ . It follows from the formulas of Section 3 that, for appropriately defined  $\chi_j^\nu$  and  $L_j^\nu$ , the substitution of the function  $\Psi = \hat{\chi}^\nu \psi^\nu$  in the original equation gives

$$ih \frac{\partial \Psi}{\partial t} - \frac{h^2}{\mu^2} \hat{\mathcal{L}} \Psi = h^2 \mu^{N-1} \hat{F} \psi^\nu + \hat{\chi}^\nu f.$$

Here  $\hat{F}$  is, in general, a pseudodifferential operator that does not change (as well as the operator  $\hat{\chi}^\nu$ ) the order of the functions  $\psi^\nu$  with respect to the parameter  $h$  if the functions oscillate with a characteristic wavelength not less than  $h$ . Applying the estimate (5.3) to this equation, we readily come to the following conclusion: the function  $\Psi$  differs from the exact solution by a value of the order  $O(h^\delta)$ ,  $\delta > 0$ , for  $h \ll 1$  or of the order  $O(\mu)$  for  $h = 1$  if  $N \geq 1$  and the discrepancy  $f$  is equal to  $O(h^{\delta+1})$  for  $h \ll 1$  or to  $O(\mu)$  for  $h = 1$ . Thus, the minimal reasonable number of terms in the expansion of the operator  $\hat{\chi}^\nu$  in constructing the semiclassical asymptotics is equal to 2 (*i.e.*, we must consider the zeroth- and first-order terms). But if we are interested in the long-wave approximation (*i.e.*, in the case  $h = 1$ ), then, obviously, in the expansion of  $\hat{\chi}^\nu$  we must consider three terms (*i.e.*,  $N = 2$ ). In this case, it suffices to solve the reduced Equation (5.2) up to  $O(\mu)$ .

The problem of calculating the symbols of the operators  $\hat{\chi}^\nu$  and  $\hat{L}^\nu$  is quite similar to problems in perturbation theory for operators with discrete spectrum (in particular, matrices), and the function  $L^\nu$  is similar to an eigenvalue, while  $\chi^\nu$  is similar to an eigenfunction. The terms of the expansion of the symbols  $\chi^\nu$  and  $L^\nu$  are calculated successively, but the explicit calculation of  $L_j^\nu$  precedes the calculation of  $\chi_j^\nu$  and is based on the fact that  $\chi_j^\nu$  exists. On the other hand, the leading term of the asymptotics is already determined by  $\chi_0^\nu$  (and, naturally, by the function  $\psi^\nu$ ). Thus, in the construction of the semiclassical asymptotics in the minimal reasonable approximation, explicit formulas are required only for  $L_0^\nu$ ,  $L_1^\nu$  and  $\chi_0^\nu$ , while in the construction of the long-wave asymptotics, explicit formulas are required for  $L_0^\nu$ ,  $L_1^\nu$ ,  $L_2^\nu$  and  $\chi_0^\nu$ ,  $\chi_1^\nu$ . Moreover, as was already discussed in Section 5.1.5 to obtain the medium-wave and long-wave approximations ( $h \gg \mu$ ), for  $L_1^\nu$ , it suffices to calculate this function and its first-order derivative for  $p = 0$ , while for  $L_2^\nu$ , it suffices to calculate this function for  $p = 0$ . This fact is very important for deriving explicit formulas. It should be noted that, although the terms  $\mu \hat{\chi}_1^\nu \psi^\nu$  for  $h \ll 1$  and  $(\mu \hat{\chi}_1^\nu + \mu^2 \hat{\chi}_2^\nu) \psi^\nu$  for  $h \sim 1$  are only corrections to the leading term  $\hat{\chi}_0^\nu \psi^\nu$  of the asymptotic expansion, it can be described correctly only if the existence of such corrections is guaranteed, while the discrepancy obtained by a direct insertion of the function  $\hat{\chi}_0^\nu \psi^\nu$  into the original equation is not sufficient to prove that the difference

between  $\hat{\chi}_0^\nu \psi^\nu$  and the exact solution is small. Here we have the following distinction from the standard semiclassical approximation for the scalar Schrödinger equation: in the latter case, the substitution of the leading term of the asymptotics in the original equation readily gives the desired small discrepancy  $O(\hbar^2)$ .

### 5.1.7. Essential part of the quantum Hamiltonian for longitudinal motion

Thus, it follows from the analysis performed in the preceding sections that, in all cases (a)–(d), the leading term of the asymptotic expansion of  $\psi^\nu$  (as well as of  $\Psi$ ) is completely determined (sometimes, with excessive accuracy) by the quantum Hamiltonian

$$\hat{\mathcal{L}}^\nu = \frac{1}{2} \left( -i\hbar \frac{\partial}{\partial x} \right)^2 + v_{\text{eff}}^1 + \frac{\hbar^2}{\mu} \left[ L_1^\nu \left( \frac{\partial}{\partial x}, \frac{\mu}{\hbar} (-i\mu \frac{\partial}{\partial x}) \right) + \mu L_2^\nu(x, 0) \right].$$

This Hamiltonian is naturally called the *essential part of the Hamiltonian of longitudinal motion on the  $\nu$ -th subband of size quantization*.

### 5.1.8. Semiclassical splitting of adiabatic terms

For  $\hbar \gg \mu$ , the correction  $L_1(x, 0)$  can change the effective Hamiltonians. This change can be essentially important for the case in which the term is degenerate or (and) the original problem is a vector problem (*i.e.*, the original quantum Hamiltonian is a matrix Hamiltonian). Let us consider this situation in more detail. Because the original problem is self-adjoint, the matrix  $L_1(x, 0)$  is Hermitian. We assume that all its eigenvalues  $\lambda_1(x), \dots, \lambda_r(x)$  are distinct and, along with the eigenvectors, smoothly depend on  $x$ . Moreover, to avoid any renormalization of energy, for simplicity, we assume that  $\lambda_j(x)$  varies along the waveguide and  $\lambda_j = 0$  at the beginning of the waveguide. Since any adiabatic term is degenerate, there is a great ambiguity in the choice of vector functions  $\chi_j^\nu, j = 1, \dots, r$ , and any variation in their choice naturally leads to a change of the matrix  $L_1^\nu$ . We choose the vector functions  $\chi_j^\nu, j = 1, \dots, r$ , so that the matrix  $L_1^\nu(x, 0)$  be diagonal. If  $1 \gg \hbar \gg \mu$  (we have the “medium-wave” approximation), the expressions  $\frac{\hbar^2}{\mu} \lambda_j(x)$  must be added to the semiclassical Hamiltonian. Following an argument similar to that in Section 5.1.2, we conclude that the parameter  $\hbar$  must satisfy the inequality  $\sqrt{\mu} \geq \hbar \gg \mu$ . We see that the semiclassical Hamiltonians (terms)  $\frac{1}{2}(p^h)^2 + v_{\text{eff}}^1 + \frac{\hbar^2}{\mu} \lambda_j$  become different for different  $j$  and thus the “semiclassical” separation of “adiabatic” terms occurs. The value of this splitting depends on  $\hbar^2/\mu$  and attains its maximum at  $\hbar \sim \sqrt{\mu}$ . In the first approximation with respect to the parameter  $\hbar^2/\mu$ , the states corresponding to different semiclassical Hamiltonians do not interact. Thus, inside an adiabatic term, we can asymptotically diagonalize the system for the vector function  $\psi^\nu$ . Although this asymptotic fact turns out to be valid for any values of  $\hbar$  from the above interval, it is clear that, for values of  $\hbar$  close to  $\mu$ , the subsequent terms of the expansion can be large, so that the above representation of such an asymptotic “diagonalization” becomes meaningless. Therefore, the situation with  $\hbar$  close to  $\mu$  must be considered as a situation with a degenerate term, and it is more natural to leave the term  $\frac{\hbar^2}{\mu} \lambda_j$  in the original correction  $\frac{\hbar^2}{\mu} L_1^\nu$ , which allows one more adequately to take into account the interaction between the states inside an adiabatic term. This reasoning concerns the case of the matrix correction  $L_1^\nu$ . In the scalar situation, the term  $\frac{\hbar^2}{\mu} L_1^\nu(x, 0)$  can always be included into the effective Hamiltonian, but, in general, this does not hold in the vector case. We have no opportunity to discuss the problems touched upon in this section in more detail. We only point out that all phenomena mentioned in this and in the preceding sections are completely determined by the essential part of the matrix analog of the Hamiltonian of longitudinal motion on the  $\nu$ th subband of size quantization.

## 5.2. ESSENTIAL PARTS OF THE EFFECTIVE HAMILTONIANS FOR LONGITUDINAL MOTIONS IN NANOTUBES FOR DIFFERENT REGIMES

The goal of this subsection is to realize the ideas from the previous subsection concerning the problem of quantum waves in nanotubes with spin taken into account.

As already noted, the “rapidity” of the longitudinal mode is determined by the parameter  $h$ . For  $h \ll 1$ , the corresponding states (in particular, the levels of longitudinal motion) are described by semiclassical asymptotics. Since a strong electric or magnetic field increases the longitudinal energy of a particle while it passes through the tube, the parameter  $h$  cannot be chosen arbitrarily and must be consistent with the strengths of the external fields contained in the problem. For mathematical rigor, we must assume that there is a functional dependence between the parameters  $\mu$ ,  $h$  and the strengths of the fields. From a physical point of view, it is natural to speak about the values of the different terms in (4.44) in their dependence on the “rapidity” of the longitudinal mode and the strengths of external fields. For a solution with wavelength  $\sim h$  to exist, it is necessary that the work of the effective field  $E_{\text{eff}}(x) = -\partial v_{\text{ext}}/\partial x - \partial \varepsilon_{\perp}(x)/\partial x - \langle \partial_x \mathbf{R}, \partial \mathbf{A}_0/\partial t \rangle$  along the tube does not exceed, in order of magnitude, the characteristic kinetic energy of the longitudinal motion:  $\varepsilon_{\parallel} \sim \mu^2/h^2$ . This implies the following constraints on the external fields and the “oscillation” in the dimensions of the section. We assume that the potential of the external electric field is equal to zero at one of the tube ends; thus,  $v_{\text{ext}}(\mathbf{R}(x), t)$  will be equal to the work of the field along the tube. This implies that the external potential in dimensionless variables has the order of  $\mu^2/h^2$ . We introduce the functions  $v_{\text{ext}}^1(x, t)$  and  $\lambda^v(x)$  determined by the relations  $v_{\text{ext}}(\mathbf{R}(x), t) = (\mu^2/h^2)v_{\text{ext}}^1(x, t)$ ,  $\varepsilon_{\perp}^v(x) = \varepsilon_{\perp}^v(0) + (\mu^2/h^2)\lambda^v(x)$  and we assume that  $v_{\text{ext}}^1(x, t)$ ,  $\lambda^v(x)$  take values that do not exceed unity with respect to the parameter.

In what follows, for simplicity, we assume that the function  $v_{\text{ext}}^1$ , in fact, smoothly depends on  $t'$ , and we write  $v_{\text{ext}}^1(x, t')$ . The constraint on the effective field implies a constraint on the character of the time-dependence of the magnetic field. We assume that  $\mathbf{H} = \mathbf{H}_0 + (\mu/h)\mathbf{H}_1(t')$ .

We replace the “adiabatic” momentum operator  $\hat{p} = -i\mu\partial/\partial x$  by the “dynamic” operator  $\hat{p}^h = -ih\partial/\partial x$ , obtain  $\hat{p} = (\mu/h)\hat{p}^h$ , and then divide the adiabatic Hamiltonian by  $\mu^2/h^2$  to “compensate” the redefined momentum. This leads to the redefined classical momentum  $p = (\mu/h)p^h$  and, by (4.44), to the following formula for the symbol  $\mathcal{L}^v(p^h, x, t', \mu, h)$  of the essential part of the quantum effective Hamiltonian  $\hat{\mathcal{L}}^v$  of the longitudinal motion:

$$\begin{aligned} \mathcal{L}^v = & \left[ \frac{(p^h)^2}{2} + v_{\text{ext}}^1(\mathbf{R}(x), t') + \phi(x, t') + \lambda^v(x) \right] E_r \otimes E_s \\ & + \frac{h^2}{\mu} \left[ -E_r \otimes \frac{1}{2} \langle \boldsymbol{\sigma}, \mathbf{H} \rangle - \frac{1}{2} \langle \partial_x \mathbf{R}, \mathbf{H} \rangle \Lambda \otimes E_s + L_{sy} \right] + h \left[ (\partial_x \Phi) \Lambda - \langle \mathbf{Y}_{\perp}, \mathbf{H} \rangle \right] \otimes E_s p^h \\ & + \mu \left\langle \mathbf{Y}, \nabla v_{\text{ext}}^1 + \frac{\partial \mathbf{A}_0^1}{\partial t'} + k(p^h)^2 \mathbf{n} \right\rangle - \frac{h^2 k(x)^2}{8} E_r \otimes E_s, \end{aligned} \quad (5.5)$$

where  $\mathbf{A}_0^1 = (1/2)[\mathbf{R}, \mathbf{H}_1(t')]$ ,  $\phi(x, t') = (1/2) \int_{x^*}^x \langle \partial_x \mathbf{R}(x'), [\mathbf{R}(x'), \partial \mathbf{H}_1(t')/\partial t'] \rangle dx'$ . Omitting the primes, we obtain the desired reduced equation on the subregion of dimensional quantization in the form:

$$ih \frac{\partial \psi^v}{\partial t} = \hat{\mathcal{L}}^v \psi^v, \quad \hat{\mathcal{L}}^v = \mathcal{L}^v \left( -ih \frac{\partial}{\partial x}, \frac{2}{x}, t, \mu, h \right). \quad (5.6)$$

Along with formulas (4.37) and (4.40), this equation, for different relations between  $\mu$  and  $h$ , determines the leading term of the asymptotic solutions of the original equation (2.2). Some-



times, several terms in (5.5) can be omitted, and several terms from the “adiabatic” correction (sometimes, matrix terms) can be transferred to the leading part of the “semiclassical” effective Hamiltonian determining, in particular, the dynamics of the classical motion of a particle in a thin tube or, if the terminology introduced in [15, 38] is used, determining the *nonstandard characteristics* of the original equation (2.2). We describe this “transfer” and the corresponding classical systems in the next subsection.

### 5.2.1. Equations of classical mechanics in nanotubes with spin and the term multiplicity taken into account

Below we perform different expansions of the function (5.5). For  $h \ll 1$ , we set  $\mathcal{L}^\nu = \mathcal{L}_0^\nu + h\mathcal{L}_1^\nu + \dots$ , where  $\mathcal{L}_0^\nu$  denotes the terms larger than  $h$  and  $h\mathcal{L}_1^\nu$  denotes the terms  $\sim h$ . According to [15, 38], these terms allow one to reconstruct the leading term of the semiclassical asymptotics completely for  $h \ll 1$ , which outside the focal points has the form of WKB-solutions  $\psi^\nu \approx \exp(iS^\nu(x, t)/h)A^\nu(x, t)$ . Their phases  $S^\nu(x, t)$  can be determined by integrating the one-dimensional Hamiltonian system

$$\dot{p}^h = \partial H_{\text{eff}}^h / \partial x, \quad \dot{x} = -\partial H_{\text{eff}}^h / \partial p^h \quad (5.7)$$

with the classical Hamiltonian  $H_{\text{eff}}^h(p^h, x)$ , which is an eigenvalue of the matrix symbol  $\mathcal{L}_0^\nu$ . If the matrix  $\mathcal{L}_0^\nu$  has distinct eigenvalues, the *semiclassical splitting of the adiabatic term* occurs, *i.e.*, several distinct classical Hamiltonians  $H_{\text{eff}}^h$  can correspond to the same adiabatic term  $H_{\text{eff}}$ . The vector part of the asymptotics  $\psi^\nu$  can be found from the linear “polarization” equation which contains  $\mathcal{L}_1^\nu$ .

We shall consider the following situations corresponding to different relations between the parameters  $\mu$  and  $h$ .

(a) *Short-wave regime:  $h = \mu$ .* Then

$$\begin{aligned} \mathcal{L}_0^\nu &= H_{\text{eff}}^h E_r \otimes E_s, \quad H_{\text{eff}}^h = \frac{(p^h)^2}{2} + v_{\text{eff}}^h, \quad v_{\text{eff}}^h = v_{\text{ext}}^1(\mathbf{R}(x), t) + \phi(x, t) + \lambda^\nu(x), \\ \mathcal{L}_1^\nu &= \left\langle \mathbf{Y}, \nabla v_{\text{ext}} + \frac{\partial \mathbf{A}_0^1}{\partial t} + k(p^h)^2 \mathbf{n} \right\rangle \otimes E_s + \left[ (\partial_x \Phi) \Lambda - \langle \mathbf{Y}_\perp, \mathbf{H} \rangle \right] \otimes E_s p^h \\ &\quad + \left[ -E_r \otimes \frac{1}{2} \langle \boldsymbol{\sigma}, \mathbf{H} \rangle - \frac{1}{2} \langle \partial_x \mathbf{R}, \mathbf{H} \rangle \Lambda \otimes E_s + L_{sy} \right]. \end{aligned} \quad (5.8)$$

The Hamiltonian system in this case is equivalent to the Newtonian system  $\ddot{x} = -\partial v_{\text{eff}}^h / \partial x$ . By the estimates in Sections 5.1.4 and 5.1.5, the leading term of the semiclassical asymptotics, which is determined by these classical equations, must give a good approximation in problems with external fields  $|\mathbf{H}| \lesssim 1$  T,  $E_{\text{ext}} = |\nabla v_{\text{ext}}| \lesssim 10^{-3}$  V/nm.

(b) *Medium-wave regime:  $h = \mu^{1/2}$ .* In this case, we have

$$\begin{aligned} \mathcal{L}_0^\nu &= \left[ \frac{(p^h)^2}{2} + v_{\text{ext}}^1(\mathbf{R}(x), t) + \phi(x, t) + \lambda^\nu(x) \right] E_r \otimes E_s + W, \\ W &= \left[ -E_r \otimes \frac{1}{2} \langle \boldsymbol{\sigma}, \mathbf{H} \rangle - \frac{1}{2} \langle \partial_x \mathbf{R}, \mathbf{H} \rangle \Lambda \otimes E_s + L_{sy} \right], \quad \mathcal{L}_1^\nu = \left( (\partial_x \Phi) \Lambda - \langle \mathbf{Y}_\perp, \mathbf{H} \rangle \right) \otimes E_s p^h. \end{aligned} \quad (5.9)$$

Thus, here the symbol  $\mathcal{L}_0^\nu$  is a matrix symbol. Here the classical effective Hamiltonians are the eigenvalues of the matrix  $\mathcal{L}_0^\nu$ . Obviously, they can be represented as the sum of the function  $(p^h)^2/2 + v_{\text{ext}}^1(\mathbf{R}(x), t) + \phi(x, t) + \lambda^\nu(x)$  and the eigenvalues of the matrix  $W$  which, in general, depend on  $p^h$ . If they are distinct for all  $(p^h, x)$ , the semiclassical splitting of the adiabatic term occurs. Obviously, these classical Hamiltonians depend on the spin terms; hence the spin

of a particle affects its phase trajectory as follows: the energy of longitudinal motion in the tube, in contrast to the total energy and the energy of transverse motion, is comparable with the spin energy.

The eigenvalues of the matrix  $W$  depend on the form of the transverse section of the tube and on the external fields. As the simplest example, we consider the case of the cylindrically symmetric crystal potential ( $y_1 = \varrho \cos \phi$ ,  $y_2 = \varrho \sin \phi$ )  $v_{\text{int}} = v_{\text{int}}(\varrho)$ , and  $w^v = \exp(\pm i v \phi) u^v(\varrho)$ . In this case,  $\mathbf{Y} = 0$ , the eigenvalues of the matrix  $\Lambda$  are  $\pm v$ ,  $M^1 = M^2 = 0$ ,  $M^0$  is the diagonal matrix with elements  $\pm \kappa v$ ,  $\kappa = 2\pi \int_0^\infty (\partial v_{\text{int}}(\varrho)/\partial \varrho) (u^v(\varrho))^2 d\varrho$ , and the adiabatic term splits into four semiclassical ones determined by the classical effective Hamiltonians  $(H_{\text{eff}}^h)_{\uparrow\downarrow}^\pm = (p^h)^2/2 + (v_{\text{eff}}^h)_{\uparrow\downarrow}^\pm$ ,

$$(v_{\text{eff}}^h)_{\uparrow\downarrow}^\pm = v_{\text{ext}}^1(\mathbf{R}(x), t) + \phi(x, t) + \lambda^v(x) \mp \frac{1}{2} \langle \partial_x \mathbf{R}, \mathbf{H} \rangle v + \sigma_{\uparrow\downarrow} \left| \frac{1}{2} \mathbf{H} \pm v \mu^{-1} \alpha \kappa \partial_x \mathbf{R} \right|, \quad (5.10)$$

where  $\sigma_{\uparrow\downarrow} = \pm 1$ . In this case, we must assume that  $|(1/2)\mathbf{H} \pm \mu^{-1}\alpha\kappa v \partial_x \mathbf{R}| \neq 0$ . Otherwise, the effect of intersection of terms or of a change in the multiplicity of the characteristics occurs, where the standard semiclassical approximation does not work (see, e.g., [4]). In this example, the Hamiltonian system is also equivalent to the Newton system with the effective potential  $(v_{\text{eff}}^h)_{\uparrow\downarrow}^\pm$ . The semiclassical approximation must work for external fields  $|\mathbf{H}| \lesssim 1$  T,  $E_{\text{ext}} = |\nabla v_{\text{ext}}| \lesssim 10^{-5}$  V/nm. We also note that (5.9) can be treated as an equation with operator-valued symbol (its operator symbol is a matrix), and we can again apply the ‘‘operator’’ reduction to this equation.

(c) *Long-wave regime:  $h = 1$ .* In contrast to the above regimes, for the ‘‘long-wave’’ approximation to exist, it is necessary to impose additional constraints on the value of the magnetic field. Formally, this follows from the existence of a term  $\sim h^2/\mu$  in the Hamiltonian (5.5). The physical cause consists in the following. Even without spin effects taken into account, the longitudinal and transverse modes are related due to the interaction between the magnetic field and the transverse orbital momentum, which is described by the term  $-(2\mu)^{-1} \langle \partial_x \mathbf{R}, \mathbf{H} \rangle \Lambda \otimes E_s$ . In this case, the transverse energy significantly exceeds the longitudinal energy; hence the dynamics of longitudinal motion becomes very sensitive to small variations in the transverse energy. In turn, the transverse energy changes because of the variation in the magnetic field flux through the tube section due to a change in the angle between the plane of the tube transverse section and the vector of the magnetic field  $\mathbf{H}$ . For the magnetic fields  $\sim 1$  T chosen above, this interaction accelerates the particle to energies that are not consistent with the parameter  $h$ . To avoid the acceleration, we must take into account that  $\varepsilon_\perp^v(x) = \varepsilon_\perp^v(0) + \mu^2 \lambda^v(x)$ , and  $\mathbf{H}_0 = 0$ ,  $\mathbf{H} = \mu \mathbf{H}_1$ . This means that we consider magnetic fields  $\lesssim 10^{-2}$  T. We also assume that the dimensionless constant of spin-orbit interaction is  $\alpha \sim \mu^2$ . This implies that the leading part of the Hamiltonian contains only the terms  $L_2^v(0, x)|_{\mathbf{H}=0, v_{\text{ext}}=0, \alpha=0}$ . Subsequent calculations of this term (see [84, Appendix A3]) lead to the last term in (5.5). As a result, we obtain the reduced limit equation of the form

$$\left[ \left( -\frac{1}{2} \frac{\partial^2}{\partial x^2} + v_{\text{ext}}^1(x) + \phi(x, t) \right) E_r \otimes E_s + (\partial_x \Phi) \Lambda \otimes E_s \left( -i \frac{\partial}{\partial x} \right) + W \right] \psi^v = 0$$

$$W = \left( \lambda^v(x) - \frac{k^2}{8} \right) E_r \otimes E_s - \frac{1}{2} \langle \partial_x \mathbf{R}, \mathbf{H}_1 \rangle \Lambda \otimes E_s - E_r \otimes \frac{1}{2} \langle \sigma, \mathbf{H}_1 \rangle + \mu^{-1} L_{sy}. \quad (5.11)$$

Here the semiclassical approximation cannot be used and any information about the solutions of the reduced equation (more precisely, about the systems of equations) can be obtained either by general qualitative methods or by numerical integration [31–36, 57, 58, 89]. As

already noted for the Helmholtz operator in plane one-mode waveguides, such an equation was first obtained in [55], where, in particular, it was proved that one can organize a single bound state in the waveguide by choosing an appropriate curvature of the waveguide. An equation similar to (5.11) and several consequences of it were obtained in [34, 35]. Equation (5.11) works in the case where the correction  $L_1^v$  is small. This imposes several constraints on the value of the constant-in-time component of the magnetic field  $H_0 \sim \mu$  and on the constant of the spin-orbit interaction  $\alpha \sim \mu^2$ .

(d) *Ultrashort-wave regime:*  $\mu^{3/2} \ll h \ll \mu$ . In the case of ultrashort-wave approximation, the external magnetic and electric fields can be stronger than those considered above. Namely,  $v_{\text{ext}} \sim \mu^2/h^2$ ,  $|\mathbf{H}(t)| \sim \mu/h$ ,  $|\mathbf{H}| \lesssim 10$  T. Introducing the notation  $v_{\text{ext}} = (\mu^2/h^2)v_{\text{ext}}^1$ ,  $\mathbf{H}(t) = (\mu/h)\mathbf{H}_1(t)$  and omitting the primes, we obtain

$$\begin{aligned} \mathcal{L}_0^v &= H_{\text{eff}}^h E_r \otimes E_s + (h^2\mu^{-2})\varepsilon_{\perp}^v(x) + \mu \left( -\langle \mathbf{Y}_{\perp}, \mathbf{H} \rangle p^h + \left\langle \mathbf{Y}, \nabla v_{\text{ext}} + \frac{\partial \mathbf{A}_0}{\partial t} + k(p^h)^2 \mathbf{n} \right\rangle \right), \\ \mathcal{L}_1^v &= \left( p^h (\partial_x \Phi) - 1/2 \langle \partial_x \mathbf{R}, \mathbf{H}_1 \rangle \right) \Lambda - 1/2 \langle \boldsymbol{\sigma}, \mathbf{H}_1 \rangle + \mu^{-1} \alpha \left( M^1 \otimes \langle \boldsymbol{\sigma}, \mathbf{n}_1 \rangle p^h + M^2 \otimes \langle \boldsymbol{\sigma}, \mathbf{n}_2 \rangle p^h \right), \end{aligned} \quad (5.12)$$

where  $H_{\text{eff}}^h = (p^h)^2/2 + v_{\text{ext}}(x) + \phi$ . Although  $\mathcal{L}_0^v$  is a matrix symbol in this case, its leading part is  $H_{\text{eff}}^h E_r \otimes E_s$ . Nevertheless, the matrix correction  $\sim \mu > h$  can lead to the splitting of the adiabatic term and, in particular, to additional terms in the phase of the wave function  $\sim \mu/h$ ,  $\mu^2/h$ ,  $\dots$ , which are, in general, different for each of the states contained inside the adiabatic term.

### 5.3. EXAMPLES OF ASYMPTOTIC SOLUTIONS FOR SOME PROBLEMS IN NANOTUBES

As we mentioned above, here we have no opportunity to describe in detail asymptotic solutions of the effective equation of adiabatic motion in nanotubes and particularly to discuss concrete physical conclusions. This discussion requires a special publication (see [85]) and probably not a single one. Here we only want very briefly to outline the structure of semiclassical asymptotics for some natural problems.

#### 5.3.1. Wave trains propagation

It is natural to formulate the problem of wave-train propagation for the reduced equation (5.6). We consider the general case when  $\mathcal{L}_0^v$  and  $\mathcal{L}_1^v$  are matrices. Let  $H_{\text{eff}}^h$  be the certain eigenvalue of the matrix  $\mathcal{L}_0^v$ . If  $H_{\text{eff}}^h$  is degenerate, to restrict on the subspace corresponding to it, we can apply the reduction of Section 3 (by parameter  $h$  instead of  $\mu$ ) once again. So we have to restrict the operator  $\mathcal{L}_1^v$  to the subspace corresponding to the eigenvalue  $H_{\text{eff}}^h$ . After the reduction our problem has the following form: the leading part of the matrix Hamiltonian is proportional to unity  $r' \times r'$ -matrix with coefficient  $H_{\text{eff}}^h$ , where  $r'$  is the multiplicity of degeneracy of eigenvalue  $H_{\text{eff}}^h$ , and  $\mathcal{L}_1^v$  is a  $r' \times r'$ -matrix. Thus we can always reduce the problem of the construction of semiclassical solutions to the problem with the leading term proportional to the unity matrix. We construct an asymptotic solution assuming that the initial problem is reduced to this form. In order to not overload the notation we will write  $\mathcal{L}_1^v$  for the matrix restricted to the proper subspace corresponding to eigenvalue  $H_{\text{eff}}^h$ .

Let  $\psi^v(x, 0) = \psi_0(x) = \exp\left(\frac{iS_0(x)}{h}\right) \varphi_0(x)$ , where the phase  $S_0(x)$  is a smooth function and  $\varphi_0(x)$  is a  $2r$ -dimensional smooth vector function of  $x \in \mathbb{R}$  with compact support  $\mathcal{M}$ . Then in the semiclassical approximation the solution to (5.6) is determined by the solution to the Hamiltonian system (5.7) with Hamiltonian  $H_{\text{eff}}^h = \frac{1}{2} p^h + v_{\text{eff}}^h$ , where  $v_{\text{eff}}^h$  depending on regimes of longitudinal motion are defined by formulas (5.8), (5.10) with initial conditions  $p^h(0) =$

$\partial S_0/\partial x(x_0)$ ,  $x(0)=x_0$ . Denote its solution by  $p^h=\pi(t, x_0)$ ,  $x=\xi(t, x_0)$ . Suppose that  $J(x_0, t)=d\xi/dx_0 \neq 0$  for  $t \in [0, t^*]$  and  $x_0 \in \mathcal{M}$ . Then the equation  $x=\xi(x_0, t)$  is uniquely solvable,  $x_0=X_0(x, t) \in \mathcal{M}$ , and, for  $t \in [0, t^*]$ , the asymptotic solution to the Cauchy problem for system (5.6) with initial condition  $\psi|_{t=0}=\psi^0(x, h)$  has the form:

$$\psi(x, t) = \left[ \exp\left(\frac{iS(x_0, t)}{h}\right) \left( \frac{\varphi(x_0, t)}{\sqrt{J(x_0, t)}} + O(h) \right) \right]_{x_0=X_0(x, t)}, \quad (5.13)$$

$$S(x_0, t) = S_0(x_0) + \int_0^t \left( \pi_i \frac{\partial H_{\text{eff}}^h(\pi, \xi, t)}{\partial \pi_i} - H_{\text{eff}}^h(\pi, \xi, t) \right) dt. \quad (5.14)$$

Function  $\varphi(x_0, t)$  satisfies the following equation:

$$\frac{d\varphi}{dt} + i\mathcal{L}_1\varphi = 0 \quad (5.15)$$

with initial condition  $\varphi(x_0, 0) = \varphi_0(x_0)$ .

For  $t > t^*$  the asymptotics of the solution is specified by use of the Maslov canonical operator  $K_{\Lambda_t}$  (see [83, 90]) on the curves  $\Lambda_t^1 = \{x = \xi(x_0, t), p = \pi(x_0, t)\}$ :  $\psi = \mathbf{K}_{\Lambda_t} \psi_0$ .

#### *Remark*

In the case of a finite effective potential the effect of splitting of the incoming wave train into two space components can appear. They are partially reflected and partially transmitted, containing harmonics  $E < \max v_{\text{eff}}^h$  and  $E > \max v_{\text{eff}}^h$ , respectively.

#### 5.3.2. Plane wave scattering

Consider a nanotube having the following structure. For  $x < x_-$  and  $x > x_+$  ( $x_{\pm} = \text{const}$ ), this tube has a rectilinear axis, constant torsion angles  $\Phi^-$  and  $\Phi^+$ , and contraction coefficients  $D_-$  and  $D_+$  at the ends. Suppose that  $\mathbf{H} = 0$ ,  $v_{\text{ext}}$  and  $v_{\text{int}}$  do not depend on  $t$ ,  $v_{\text{ext}}(\mathbf{R}(x)) = \{v_{\text{ext}}^- \text{ for } x < x_-, v_{\text{ext}}^+ \text{ for } x > x_+\}$ ,  $v_{\text{int}}(x, y) = \{v_{\text{int}}^-(y) \text{ for } x < x_-, v_{\text{int}}^+(y) \text{ for } x > x_+\}$ . Then for  $x < x_-$  and  $E > v_{\text{ext}}^- + \varepsilon_-^v$ , the system has a solution of the form  $\exp((-iEt + ip_-x)/h)g_-^{vk}(y)$ ,  $k=1, \dots, 2r$ , which represents a plane wave propagating along the tube axis with vector (spinor) amplitude  $g_-^{vk}(y)$ . Vector  $g_-^{vk}(y)$  and  $\varepsilon_-^v$  are the eigenfunction and eigenvalue of the following problem, correspondingly:

$$\left( -\frac{1}{2} \frac{\partial^2 g}{\partial y^2} + v_{\text{int}}^-(y) + \alpha(\boldsymbol{\sigma}, \hat{\mathbf{M}}) \right) g_-^{vk}(y) = \varepsilon_-^v g_-^{vk}(y), \quad \mathbf{n}_0 = \partial_x \mathbf{R}, \quad (5.16)$$

$$\hat{\mathbf{M}} = \partial_x \mathbf{R} \left( (\partial_1 v_{\text{int}}) \partial_2 - (\partial_2 v_{\text{int}}) \partial_1 \right) + \mathbf{n}_1 (\partial_2 v_{\text{int}}) p - \mathbf{n}_2 (\partial_1 v_{\text{int}}) p. \quad (5.17)$$

#### *Remark*

Note that the eigenfunction  $g^{vk}$  is not the product  $w_j^v(y) \otimes \eta$  of “pure state” inside the term  $w_j^v(y)$  and “pure spin state”  $\eta_k$  ( $\eta_k$  does not depend on  $y$ ). This means that we cannot separate spin states and states inside one term. Since the parameter  $\alpha \ll 1$ , to construct  $g^{vk}$  one can use perturbation theory. To construct solutions in the case when  $v_{\text{int}} = y_1^2 + y_2^2$  (parabolic confinement) one has to use second-order perturbation theory.

As exact solutions “at infinity” are not products of “pure states,” we need to expand them with respect to the basis  $w_j^v(y) \otimes \eta^k$ . We obtain:

$$g_-^{vk}(y) = \|w_1^v(y), \dots, w_r^v(y)\| \otimes E_s \varphi^-, \quad \varphi^- = \{\varphi_1^-, \dots, \varphi_{2r}^-\}^T. \quad (5.18)$$

The evolution of “initial scattering data” for the reduced equation is determined by the following transport equation:

$$\frac{d\varphi}{dt} + i\mathcal{L}_1^v\varphi = 0, \quad \varphi \rightarrow \varphi^-, \quad t \rightarrow -\infty. \quad (5.19)$$

The final scattering data for the reduced equation is  $\varphi^+ = \lim_{t \rightarrow \infty} \varphi(t)$ . So we obtain the final scattering data for the original problem in the form:

$$g_+^{vk'}(y) = \|w_1^v(y), \dots, w_r^v(y)\| \otimes E_s \varphi^+. \quad (5.20)$$

In the semiclassical approximation this problem has a  $2r$ -dimensional family of asymptotic solutions of the form  $\psi(x, E) \simeq \mathbf{K}_{\Lambda^1(E)}\{\varphi(t)\}$ , where  $\mathbf{K}_{\Lambda^1(E)}$  is the Maslov canonical operator on the nonclosed curve  $\Lambda^1(E) = \{H_{\text{eff}}^h = E : p^h = p^h(t), x = x(t)\}$ ,  $t$  is the proper time (parameter on  $\Lambda^1(E)$ ):  $dx/dt = \pm \sqrt{2(E - v_{\text{eff}}^h(x))}$ . Let  $E > v_{\text{eff}}^h(x)$  for each  $x$ . Then with an accuracy exponential with respect to  $h \rightarrow 0$ , we have a passage of the incident wave above the barrier; as  $x \rightarrow \pm\infty$

$$\psi(x, E, h) \rightarrow \frac{1}{\sqrt{p_{\pm}}} \exp\left(\frac{i}{h} p_{\pm} x\right) \varphi^{\pm}, \quad p_{\pm} = \sqrt{2(E - v_{\text{ext}}^- - \varepsilon_-^v)}. \quad (5.21)$$

If  $E < \max v_{\text{eff}}^h(x)$  at some points of the tube axis, the incident wave is reflected off the barrier with an accuracy exponential with respect to  $h$ . In the domain  $x < x_f(E)$ , where  $x_f$  is the rotation point at the energy level  $E = v_{\text{eff}}^h(x_f(E))$ ,  $\psi(x, E, h)$  is the sum  $\psi_- + e^{-i\pi/2}\psi_+(x, E, h)$  of the incident and reflected waves  $\psi_{\pm}(x, E, h)$  with  $x < x_f(E)$  (at  $x > x_f(E)$   $\psi(x, E, h) = O(h^\infty)$ ). As  $x \rightarrow -\infty$ , we have

$$\psi_{\pm} \rightarrow \frac{1}{\sqrt{p}} \exp\left(\pm \frac{i}{h} p x\right) \varphi^{\pm}. \quad (5.22)$$

The form of the nanotube after barrier modulo exponentially small corrections does not influence the solution. Therefore, the part of the tube behind the barrier can be removed. One can see from the formulas (4.42) that the barrier appears not only because of the external potential but also because of the narrowing of the tube ( $D(x) \rightarrow 0$ ). Thus the constructed asymptotics model the situation when the end of the tube narrows conically-like, which results in the appearance of a barrier, that is, a turning point in the system (5.6). It results in a sharp increase of the wavefunction in the neighborhood of the conical end of the tube; this is probably related to the effect of the luminosity of the tube end.

### 5.3.3. Bound states. Asymptotic eigenvalues

Suppose that the potential  $v_{\text{ext}}$  and the magnetic field  $\mathbf{H}$  do not depend on  $t$  and that the effective potential  $v_{\text{eff}}^h(\mathbf{R}(x))$  has a stable minimum point  $x_0$ . In its neighborhood  $v_{\text{eff}}^h(\mathbf{R}(x))$  has the form of a potential well, which generates a family of  $T(E)$ -periodic trajectories  $\xi(t, E)$ ,  $\pi(t, E)$  of system (5.7) parametrized by the energy  $E = \frac{(p^h)^2}{2} + v_{\text{eff}}^h(x)$ . Substituting them in (5.15), we obtain a system of the form  $\dot{\varphi} = -G(t)\varphi$  with a unitary matrix that is  $T$ -periodic with respect to  $t$ . We can form a basis in the space of their solutions from vectorfunctions of the form  $z^j(t, E) \exp(i\beta^j(E)t)$ , where  $j = 1, 2, \dots, 2r$ ,  $z(t, E)$  are  $T$ -periodic in  $t$ , and the Floquet exponents  $\beta^j(E)$  are real for all  $E$ . We choose them in such a way that  $|\beta^j|$  are minimal. Let  $E^{vn}$  be the levels determined by the Bohr-Sommerfeld quantization condition

$$\frac{1}{2\pi} \oint \pi d\xi = \frac{1}{\pi} \int_{x_{\min}}^{x_{\max}} \sqrt{2(E - v_{\text{eff}}^h)} dx = h \left( n + \frac{1}{2} \right), \quad n = 0, 1, 2, \dots \quad (5.23)$$

Then the values numbers  $E_j^{vn} = E^{vn} + h\beta^j(E^{vn})$ , where  $j = 1, 2, \dots, 2r$ , yield a spectral series (sets of bound states) of the operator  $\hat{\mathcal{L}}$ ; the  $O(h^2)$ -neighborhood of  $E_j^{vn}(h)$  necessarily contains a point of its spectrum (continuous or discrete). Namely, if the spectrum of the original problem on the interval  $E_0 - \varepsilon, E_0 + \varepsilon$  is discrete, then the numbers  $E_j^{vn}$  give the asymptotics of some of its eigenvalues. If the spectrum on this interval is continuous, these functions apparently approximate the exponentially small bands of the spectrum (*c.f.* [91]).

The eigenfunctions corresponding to  $E_j^{vn}(h)$  are determined by use of the Maslov canonical operator.

#### 5.4. REMARK ON THE RIGOROUS JUSTIFICATION OF THE CONSTRUCTED ASYMPTOTIC SOLUTIONS

It is natural to discuss the important question about the strict justification of asymptotic solutions, which can be constructed by using the formal procedures suggested above. In this paper, we hardly touch upon this problem (see Section 5.1) whose general solution is not trivial and requires further investigation. To study this problem, one can use at least two possible methods.

- (1) One has to prove that the asymptotic solutions are close to the exact solution of the initial problem under some conditions on the coefficients of the initial equation and on the function classes to which the solutions of the reduced equation belong. This method is based on the technique of obtaining a series of estimates with respect to the parameters  $\mu$  and  $h$  from different diapasons.
- (2) The second method of justification is to estimate the accuracy of the functions obtained, which approximate the exact solution of the initial equation. This method seems to be more useful, at least from a pragmatic point of view, since the obtained explicit asymptotic formulae for the solutions of real physical problems can be used.

#### 5.5. SEVERAL EFFECTS IN NANOTUBES GENERATED BY THEIR GEOMETRY AND EXTERNAL FIELDS

Finally let us described very briefly several effects which one can obtain from the analysis of the asymptotic solutions constructed above. (Some of them have already been discussed in Section 5.1).

##### 5.5.1. *The possibility to model effective one-dimensional potentials*

First let us mention some elementary, but curious, properties of the above equations, which are caused by the possibilities of nanotechnology: *changing the geometry of a tube placed in a homogeneous electric field, one can model different one-dimensional effective potentials.*

First, we consider a tube of constant cross-section whose axis is a plane curve in the plane  $(r_1, r_2)$ . Let an electric field of strength  $E_{\text{ext}}$  be directed along the  $Ox_2$  axis. Then the effective potential has the form  $\varphi = v_{\text{ext}}(\mathbf{R}(x)) = E_{\text{ext}}R_2(x)$ . If the tube is only slightly curved with respect to the axis  $r_1$ , then we have  $x \approx r_1$ . Thus, choosing the tube axis as an appropriate curve  $r_2 = r_2(r_1)$ , we can model the potential, the double potential well, etc.

As an example of a nonplanar tube, we consider the spiral  $\mathbf{R}(x) = (\rho_1 \cos(x/\sqrt{\rho_1^2 + \rho_2^2}), \rho_1 \sin(x/\sqrt{\rho_1^2 + \rho_2^2}), \rho_2 x/\sqrt{\rho_1^2 + \rho_2^2})$  ( $\rho_1 = \text{const}$ ,  $\rho_2 = \text{const}$  are parameters) in the field  $E_{\text{ext}}(0, \sin \alpha, \cos \alpha)$ . The effective potential contains the *oscillating and linearly increasing* components:  $\varphi(x) = -\sin \alpha E_{\text{ext}} \rho_1 \sin(x/\sqrt{\rho_1^2 + \rho_2^2}) - x \cos \alpha E_{\text{ext}} \rho_2/\sqrt{\rho_1^2 + \rho_2^2}$ . If  $\alpha = \pi/2$ , *i.e.*, the field is perpendicular to the tube axis, then we obtain a periodic potential and the equations obtained above coincide with the Mathieu equation in the first approximation. If  $\alpha = 0$ , *i.e.*, the field is directed along the tube, we obtain the Airy equation. A more complicated example is the case in which the tube axis is a winding of a torus: in this case, in particular, we can

obtain almost periodic potentials. Similar results can be obtained by changing the thickness of the tube along the tube axis.

5.5.2. *Dependence of the effective one-dimensional potential on the tube thickness*

It is easy to show that for the above potentials modelling the “soft” and “rigid” walls, the effective one-dimensional potential of the longitudinal motion depends on the tube thickness  $d_0(x)$  as  $1/d_0(x)^2$ . This dependence is a pure quantum effect which is caused by size quantization. Thus, narrowing the tube, we obtain a barrier in the one-dimensional motion, while expanding the tube, we obtain a potential well or “trap.”

5.5.3. *Semiclassical splitting of the adiabatic term*

The “adiabatic” terms can split in the semiclassical approximation due to spin and the magnetic field. In particular, if the splitting is caused by spin effects, then spin affects the “classical” trajectory. For the case in which the adiabatic term is nondegenerate, we have  $\Lambda = 0$ . If degeneration exists, the momentum matrix  $\Lambda$  is nonzero. This results in the appearance of an effective “dipole” that interacts with the projection of the magnetic field on the tube axis, and thus an additional phase of the wave function (the Berry phase) appears.

5.5.4. *An increase in the electron density near the endpoint of the nanotube caused by reflection.*

Since the longitudinal energy decreases with decreasing cross-section of the nanotube, in a nanotube with a “closed” endpoint, the wave packet reflects from the closed endpoint. In this case, near the endpoint of the nanotube, there is a sharp increase in the electron density, which, apparently, is related to the effect of luminous emittance observed in nanotubes.

5.5.5. *The Berry phase of the wave function*

The term  $[\Phi_x \Lambda - \langle Y_2 \mathbf{n}_1 - Y_1 \mathbf{n}_2, \mathbf{H} \rangle] \otimes E_s p^h$  in the Hamiltonian (5.5) proportional to the momentum  $p^h$  can be excluded from this Hamiltonian by a change of the wave function. This change has the form

$$\psi^j = \exp \left( \int_{x^*}^x \lambda_j(x) dx \right) \psi'^j, \tag{5.24}$$

where  $\lambda_j(x)$  is an eigenvalue of the matrix  $\Phi_x \Lambda - \langle Y_2 \mathbf{n}_1 - Y_1 \mathbf{n}_2, \mathbf{H} \rangle$ . In fact, the existence of this term results in the appearance of an additional phase of the wave function. This phase must be consistent with the boundary conditions at the endpoints of the tube, which gives a correction to the quantization condition. For example, we consider the Born–Kármán boundary conditions that are equivalent to the case of a closed tube (the nanoannulus). While constructing the eigenfunctions in this case, it is necessary to require that the total phase of the wave function be  $2\pi$ -periodic, with the above adiabatic correction taken into account. It is well known that the adiabatic phase responsible for the correction to the quantization condition is the so-called Berry phase.

If the magnetic field is zero, the Berry phase is reduced to  $\exp \left( \int_{x^*}^x \Lambda_j(x) d\Phi \right)$ , where  $\Lambda_j(x)$  is an eigenvalue of the momentum matrix  $\Lambda$ .

5.5.6. *Ultrashort modes and the state density*

The correction to  $\mu \chi_1$  becomes comparable with 1 for  $h = \mu^{3/2}$ . This means that the adiabatic asymptotics of the form (4.37) ceases to hold. However, for  $h < \mu$  and for the same total energy, there exists a state of the form (4.37) that belongs to the next subregion of the trans-

verse quantization. From a physical standpoint, the fact that there is no asymptotic solution of the form (4.37) in the case of ultrashort waves in a curved tube means that such fast modes are destroyed in passing from a straight tube to a curved tube; they “fall” to the next subregions because of the interaction with the tube “walls.”

The “instability” of ultrashort modes with parameter  $h < \mu^{3/2}$  in a curved tube can lead to a change in the density of states and, in contrast to the straight nanotube, effectively increase the Fermi level (*cf.* [92]).

### 5.5.7. *Spin beats*

The operator  $L_{sy}$  in the semiclassical Hamiltonian, which corresponds to spin-orbit interaction, leads to a splitting of the adiabatic term into  $2r$  semiclassical terms of the longitudinal motion. To each of the semiclassical terms, there corresponds, in general, its own phase  $S_j^v(x, t)$ ,  $j = 1, \dots, 2r$ . If the variation in the phase due to the spin-orbit interaction is small, the phase can be expanded in a series in the constant of spin-orbit interaction  $\alpha$ . The zero term in the expansion corresponds to the classical motion of a “spinless” particle, and the correction results in the appearance of an envelope for the fast-oscillating exponential. Apparently, the appearance of such an envelope is related to the observed effect of the electron density beating along the tube [93].

## 6. Concluding remarks

Let us briefly summarize the results of this paper, sometimes repeating the above arguments. The adiabatic approximation is one of the main tools for analyzing the solutions of linear stationary and nonstationary problems in modern mathematical and theoretical physics. Different versions of adiabatic approximation are used in problems of molecular physics, solid-state physics, plasma physics, theory of internal and surface waves in fluids, averaging theory, quantum gravitation theory, etc.

The adiabatic approximation is used in situations in which the study of some classes of physically interesting wave processes described by a “large” system with  $N$  degrees of freedom can be reduced, on some time intervals, to the study of a simplified “effective” system with  $n < N$  degrees of freedom. In this case, on the one hand, a sufficiently wide range of states and solutions with some general characteristic properties (but not a set of individual concrete states or solutions) is considered, and, on the other hand, it is not assumed that all the solutions of the original “large” system can be described in the same way. From a physical point of view, this possibility is usually ensured by the fact that the problem has different spatial or spatio-temporal scales, which, from a mathematical point of view, means that there is a small parameter characterizing the different scales of the problem. As a rule, the different scales are manifested in different dependences of the coefficients of the original equation or boundary conditions on various variables (or groups of variables), *i.e.*, on  $(N - n)$  “fast” and  $n$  “slow” variables. Thus, it is natural to divide the study of such distinguished wave processes into two stages: (1) to derive “effective” reduced systems, (2) to find their concrete solutions and then to reconstruct the total solution describing the entire process. Of course, these considerations appear in different fields of physics and mechanics; the problem is to realize them in concrete formulas. Moreover, in each field, its own terminology is used. For example, such reduced systems correspond to terms in molecular physics, to modes in hydrodynamic problems, to subbands of dimensional quantization in nanophysics, etc. For various reasons, it is convenient for us to use the terminology accepted in physics of low-dimensional systems.



In turn, roughly speaking, the idea to derive simplified systems has two stages: (1) first, after the  $n$  above-mentioned degrees of freedom are “frozen” (it is assumed that the differentiation operators with respect to the slow variables commute with the slow variables), the operator determining the effective equation can be obtained as an eigenvalue of an auxiliary spectral problem with  $N - n$  degrees of freedom; realizing this stage, we obtain effective Hamiltonians (or dispersion relations), well-known in molecular physics; (2) the operator (the “quantization” or the Peierls substitution) determining the effective reduced equation with  $n$  degrees of freedom is reconstructed simply by taking into account the fact that the differentiation operator with respect to slow variables does not actually commute with the slow variables. We note that the distinguishing of the “frozen” (slow) variables can be natural and obvious as, for example, in problems of molecular physics or in mechanical problems with different spatial scales, but can be more “latent” as in electron waves in crystals and in the averaging theory. In this case, an additional degree of freedom appears in the regularization of the problem.

In some problems, it is sufficient to perform the “naive” quantization of the effective Hamiltonian (of the dispersion relation), but, in many problems, a more accurate analysis is required and certain difficulties arise (see, *e.g.*, [5, Section 56]. We note that, as a rule, it is impossible to write the effective reduced equation exactly; the problem is to construct a minimally reasonable number of terms in the expansion of the operator in the effective reduced system, which allows a correct construction of the equation describing a wide range of wavelengths. Indeed, the most popular approach in the adiabatic approximation, originating from the work of Born and Oppenheimer, is based on the assumption that the desired solution depends smoothly on all the variables. Thus, for example, only the lower energy levels are usually “grasped” in spectral problems. At the same time, in many physical situations, for example, in describing the valence electrons in crystals, the higher energy levels are most interesting, but, strictly speaking, they cannot be considered under this approach. In this case, one can use the semiclassical theory proposed by Maslov, which, however, is based on the assumption that there is a sufficiently rigid relation between the excitation level and the parameter characterizing the different scales of the problem. From a mathematical point of view, this means that, in the problem under study, along with the parameter characterizing the different scales, which is naturally called an adiabatic parameter, there is another (“semiclassical”) parameter characterizing the excitation level of the state under study; in this case, the form of the approximate (asymptotic) solution depends, as a rule, on the relations between these parameters. This can easily be verified by comparing the averaging method, the Born–Oppenheimer method, and the Maslov method, which give solutions with “slow,” “medium,” and “fast” variations (with respect to the slow variables).

In this paper, we propose an approach based on the above considerations. This approach allows one, first, to describe all the states listed above, in the range from slowly varying states to fast or, sometimes, even “superfast” varying states, and, second, to classify them appropriately. In particular, this approach explains why the states obtained by the Born–Oppenheimer and Maslov methods can be treated as the states on the same subregions (terms) corresponding to different “longitudinal states.” So the effective reduced equation thus obtained describes not only the states at the “bottom” of the subregion, but also the states corresponding to the higher energy levels. We note that, without this reduction, choosing the subregion for higher energy levels can be a rather complicated problem in itself.

The approach proposed here is based on Maslov’s observation that the problems in which the adiabatic approximation is used can be interpreted as problems with operator-valued symbol, and these problems are well known in mathematical physics. This means that the

operator determining the original “large” system is a function of two groups of operators with “small” and “large” commutators (or “large” anticommutators, as in the electron-phonon interaction problem). The use of the concept proposed in this paper, which is based on equations with operator-valued symbol, allows one to deal with different linear adiabatic problems from a unified point of view.

The realization of our approach is based on representing the solution in the form (3.5) and obtaining the effective reduced equation (3.7), which is a generalization of the Peierls substitution. These formulas, together with the algorithm described in Section 3, give one of the main results of the present paper. In these constructions, the key role is played by the techniques of noncommuting operators based on elementary notions from the Maslov operator method. The constructed algorithm allows us, with any prescribed accuracy, to calculate the operator determining the effective reduced equation (3.7) and the intertwining operator reconstructing the solution of the original problem from the solution of Equation (3.7). In particular, the algorithm thus constructed allows one to obtain accurate estimates for the minimal number of terms necessary to construct the leading part of the asymptotic solution. It should be noted that, in the reduction procedure, the possible degeneration of the term (the effective Hamiltonian) must be taken into account. In Sections 4–5, these formulas are illustrated by several examples from different fields of physics and mathematics. Some heuristic arguments leading to formulas (3.5) and (3.7) are given in Section 2.

In Section 3, we also show that the “operator separation” of variables can be treated as a “quantum” (or wave) analog of the procedure of excluding (holonomic) constraints in classical mechanics ([36, 37] and others). Indeed, the imposed quantum constraints can be treated as restrictions arising due to the confinement potential in the ambient configuration space. In this case, it is natural to assume that the “condition of dimensional quantization” is satisfied, *i.e.*, the wavelength in the directions normal to the manifold corresponding to the degrees of freedom of the effective system (*i.e.*, the “limit” manifold) is compatible with the “width of the film” surrounding the limit manifold. Here the most important is the fact justified in this paper that, excluding the constraints, one can, in general, obtain different effective Hamiltonians depending on the energy of the “longitudinal” motion. In the case of fast oscillating longitudinal states, this leads to different classical Hamiltonians determining the motion on the “limit manifold.”

The study of solutions of reduced equations on some distinguished subregions has been the second part of our approach. Depending on the relations between the parameters, this study can generally be performed by different methods. In Section 5, taking into account the fact that the problem contains two parameters, an adiabatic and a semiclassical, we classify the solutions, and this classification shows that the excited states are constructed differently than the lower states. In the construction of excited states, the momentum in the intertwining operator cannot be neglected, *i.e.*, the intertwining operator is *indeed an operator* and cannot be replaced by a function, as it is usually done in different versions of the Born–Oppenheimer method (in particular, in solid-state physics). The existence of the momentum operator in the intertwining operator shows that, from the viewpoint of the Born–Oppenheimer method for excited states, a “distortion” of the term occurs. For fast varying solutions, the main methods in this case are the semiclassical approximation and the WKB-method; if there are turning points and caustics, the WKB–Maslov method is used. It is well known that, when applying this method, one must pass to classical Hamiltonian systems. One of the elementary, but important, consequences is the fact that the classical systems can be different for different excitation levels and the “small” terms in the original equation can significantly affect the semiclassical characteristics for some values of the longitudinal energies. In particular, in the

case of a degenerate adiabatic effective Hamiltonian, the degeneration can be removed in the semiclassical approximation; in this case, the adiabatic term “splits” into several semiclassical terms (Hamiltonians). We have considered an example (nanotubes) and have shown that the interaction of spin with the confinement potential can change the classical trajectories of the longitudinal motion.

As was already noted, the possibility to obtain numerical solutions, graphs, etc. at this stage significantly depends on the specific character of a concrete problem and requires separate publications. In the present paper, we briefly describe this procedure for problems related to the modern field of nanophysics and restrict ourselves to rather general formulas. In Section 5, we have derived some simplest conclusions for models arising in nanophysics. In particular, we showed that, placing nanotubes of various geometry in a constant electric field, we can model various one-dimensional potentials, for example, “double well” type potentials, periodic potentials, etc.; the degenerate adiabatic term (for example, in the case of a tube of circular cross-section) can split into several semiclassical terms (effective Hamiltonians), etc. The problems concerning detailed studies of how the spin affects classical trajectories, the electron-density pulsation due to spin, etc. are beyond the scope of this paper.

We believe that the arguments and formulas given in this paper can be helpful in studying problems arising in solid-state physics, hydrodynamics (waves on water), the theory of shells, plates, and rods, and in nanophysics. It seems possible that this method can be used in weakly nonlinear situations.

In conclusion, we make a remark concerning the list of references. As was already noted, the number of works dealing with the adiabatic approximation and its applications is very extensive; our list of references does not absolutely pretend to be complete; here we present only several papers that are to some extent close to our approach.

## Acknowledgments

The authors are grateful to S. Albeverio, J. Brüning, V.A. Geyler, K.V. Pankrashkin and I.V. Tyutin for useful discussions and valuable remarks. The work is supported in part by grants INTAS (00-257) and DFG-RAS (DFG 436 RUS 113/785, DFG 436 RUS 113/572/0-2).

## References

1. M. Born and J.R. Oppenheimer, Zur quantentheorie der molekeln. *Annalen der Physik* 84 (1927) 457–484.
2. R.E. Peierls, *Quantum Theory of Solids*. Oxford: The Clarendon Press (1955) viii + 229 pp.
3. M. Born and K. Huang, *Dynamical Theory of Crystal Lattices*. Oxford: The Clarendon Press (1954) xii + 420 pp.
4. L.D. Landau and E.M. Lifshitz, *Quantum Mechanics (Nonrelativistic Theory)*. *Theoretical Physics* 3. Moscow: Nauka (1989) 768 pp. (in Russian) L.D. Landau and E.M. Lifshitz, *Quantum Mechanics: (Nonrelativistic Theory)*. In: *Theoretical Physics* 3. Oxford, London, Edinburgh: Pergamon Press (1965) ix + 616 pp.
5. E.M. Lifshitz and L.P. Pitaevskii, *Statistical Physics. Pt. 2. Theory of Condensed State*. *Theoretical Physics IX*. Moscow: Nauka (1978) 448 pp; E.M. Lifshitz and L.P. Pitaevskii, *Statistical Physics. Pt. 2. Theory of Condensed State*. In: L.D. Landau, E.M. Lifshitz and L.P. Pitaevskii (eds.), *Course of Theoretical Physics* 9. Oxford, London, Edinburgh: Pergamon Press (1980) x + 387 pp.
6. V.P. Maslov, *Perturbation Theory and Asymptotic Methods*. Moscow: Moscow Univ. Publ. (1965) 549 pp; V.P. Maslov, *Théorie des perturbations et méthodes asymptotiques*. Paris: Dunod, Gauthier-Villars (1972) xii + 384 pp.
7. M.V. Berry, Quantal phase factors accompanying adiabatic changes. *Proc. R. Soc. London A*392 (1984) 45–57.
8. I.C. Percival, Semiclassical theory of bound states. *Adv. Chem. Phys.* 36 (1977) 1–61.
9. G.A. Hagedorn, A time dependent Born–Oppenheimer approximation. *Comm. Math. Phys.* 77 (1980) 1–19.

10. Yu.Z. Miropol'sky, *The Dynamics of Internal Gravity Waves in Ocean*. Leningrad: Gidrometeoizdat (1981) 302pp; Yu.Z. Miropol'sky, *The Dynamics of Internal Gravity Waves in Ocean*. In: *Atmospheric and Oceanographic Sciences Library* 24. Dordrecht etc.: Kluwer Academic Publishers (2001) xvii+406pp.
11. S.Yu. Dobrokhotov, Maslov's methods in linearized theory of gravitational waves on the liquid surface. *Dokl. Akad. Nauk SSSR* 269 (1983) 76–80; S.Yu. Dobrokhotov, Maslov's methods in linearized theory of gravitational waves on the liquid surface. *Sov. Phys. – Dokl.* 28 (1983) 229–231.
12. S.Yu. Dobrokhotov, Applications of Maslov's theory to two problems for equations with operator-valued symbols. (in Russian) *Usp. Mat. Nauk* 39 (1984) 125.
13. L.V. Berlyand and S.Yu. Dobrokhotov, "Operator separation of variables" in problems of short-wave asymptotics for differential equations with rapidly oscillating coefficients. *Dokl. Akad. Nauk SSSR* 296 (1987) 80–84; L.V. Berlyand and S.Yu. Dobrokhotov, "Operator separation of variables" in problems of short-wave asymptotics for differential equations with rapidly oscillating coefficients. *Sov. Phys. – Dokl.* 32 (1987) 714–716.
14. V.P. Maslov, *Operational Methods*. Moscow: Nauka (1973) 544pp; V.P. Maslov, *Operational Methods. Transl. from the Russian*. Moscow: Mir Publishers (1973) 559pp.
15. V.P. Maslov, Nonstandard characteristics in asymptotic problems. *Uspekhi Mat. Nauk* 38 (1983) 3–36; V.P. Maslov, Nonstandard characteristics in asymptotic problems. In: *Proceedings of the International Congress of Mathematicians (Warsaw, Aug. 16–24 1983)* 1, 2. Warsaw: PWN (1984) pp.139–183.
16. L.I. Schiff, *Quantum Mechanics*. New York–Toronto–London: McGraw-Hill Book Co., Inc. (1955) xii+417pp.
17. V.V. Belov, Semiclassical energy levels of a two-atom molecule in a magnetic field. *Izv. vuzov. Matematika* 6 (1976) 13–18 (in Russian).
18. G. Panatti, H. Spohn and S. Teufel, Effective dynamics for Bloch electrons: Peierls substitution and beyond. *Comm. Math. Phys.* 242 (2003) 547–578.
19. S.Yu. Dobrokhotov and P.N. Zhevandrov, Asymptotic expansions and the Maslov canonical operator in the linear theory of water waves. I. Main constructions and equations for surface gravity waves. *Russ. J. Math. Phys.* 10 (2003) 1–31.
20. S.Yu. Dobrokhotov, *Many-Phase Asymptotic Solutions to Linear and Nonlinear Partial Differential Equations with a Small Parameter*. Doctoral thesis. (in Russian). Moscow: IPMekh Akad. Nauk SSSR (1988) 293pp.
21. M.V. Karasev and V.P. Maslov, Asymptotic and geometric quantization. *Usp. Mat. Nauk* 39 (1984) 115–173; M.V. Karasev and V.P. Maslov, Asymptotic and geometric quantization. *Russ. Math. Surveys* 39 (1984) 133–205.
22. M.V. Karasev and V.P. Maslov, *Nonlinear Poisson Brackets. Geometry and Quantization*. Moscow: Nauka (1991) 366pp; M.V. Karasev and V.P. Maslov, *Nonlinear Poisson Brackets. Geometry and Quantization*. In: *Transl. Math. Monographs* 119. Providence, Rhode Island: AMS (1993) xi+366pp.
23. D.V. Anosov, Averaging in systems of ordinary differential equations with rapidly oscillating solutions. (in Russian) *Izv. Akad. Nauk SSSR. Ser. Mat.* 24 (1960) 721–742.
24. V.I. Arnold, V.V. Kozlov and A.I. Neishtadt, *Mathematical Aspects of Classical and Celestial Mechanics*. In: V.I. Arnold (ed.), R.V. Gamkrelidze (ed.-in-chief), *Progress in Science and Technology. Current Problems in Mathematics. Fundamental Directions 3 (Dynamical Systems III)*. Moscow: VINITI AN SSSR (1985) 304pp; V.I. Arnold, V.V. Kozlov and A.I. Neishtadt, *Mathematical Aspects of Classical and Celestial Mechanics*. In: V.I. Arnold (ed.), R.V. Gamkrelidze (ed.-in-chief), *Encyclopaedia of Mathematical Sciences 3 (Dynamical Systems III)*. Berlin etc.: Springer-Verlag (1988) xiv+291pp.
25. P. Lochak and P. Meunier, *Multiphase Averaging for Classical systems*. In: S.S. Antmann, J.E. Marsden and L. Sirovich (eds.), *Applied Mathematical Sciences* 72. Berlin etc.: Springer-Verlag (1988) xi+360pp.
26. A.I. Neishtadt, Averaging in multi-frequency systems. II. *Dokl. Akad. Nauk SSSR. Mekhanika* 226 (1976) 1295–1298; A.I. Neishtadt, Averaging in multi-frequency systems. II. *Sov. Phys. – Dokl.* 21 (1976) 80–82.
27. A.I. Neishtadt, The separation of motions in systems with rapidly rotating phase. *J. Appl. Math. Mech.* 48 (1984) 133–139.
28. K. Stefanski and H.C. Taylor, New approach to understanding quasiperiodicity in nonintegrable Hamiltonian systems. *Phys. Rev. A* 31 (1985) 2810–2820.
29. M.V. Berry, Classical adiabatic angles and quantal adiabatic phase. *J. Phys. A: Math. Gen.* 18 (1985) 15–27.
30. B. de Witt, Dynamical theory in curved spaces. I. Review of the classical and quantum action principles. *Rev. Mod. Phys.* 29 (1957) 377–397.
31. H. Jensen and H. Koppe, Quantum mechanics with constraints. *Ann. Phys.* 63 (1971) 586–591.
32. R.C.T. da Costa, Quantum mechanics of constrained particle. *Phys. Rev. A* 23 (1981) 1982–1987.

33. R.C.T. da Costa, Constraints in quantum mechanics. *Phys. Rev. A* 25 (1982) 2893–2900.
34. M.V. Entin and L.I. Magarill, Electrons in a twisted quantum wire. *Phys. Rev. B* 66 (2002) 205308 (5 pages).
35. L.I. Magarill and M.V. Entin, Electrons in curvilinear quantum wire. *Zh. Exper. Teor. Fiz.* 123 (2003) 867–876; L.I. Magarill and M.V. Entin, Electrons in curvilinear quantum wire. *J. Exper. Theor. Phys.* 96 (2003) 766–774.
36. P.C. Schuster and R.L. Jaffe, Quantum mechanics on manifolds embedded in Euclidean space. *Ann. Phys.* 307 (2003) 132–143.
37. V.I. Arnold, *Mathematical Methods of Classical Mechanics*. Moscow: Nauka (1974) 432pp; V.I. Arnold, *Mathematical Methods of Classical Mechanics*. In: S. Axler, F.W. Gehring and K.A. Ribet (eds.), *Graduate Texts in Mathematics* 60. Berlin etc.: Springer-Verlag (1978) x+462pp.
38. V.P. Maslov, The characteristics of pseudodifferential operators and difference schemes. In: *Actes du Congrès Internationales des Mathématiciens (Nice, 1970)* 2. Paris: Gauthier-Villars (1971) pp.755–769.
39. V.P. Maslov, *Mathematical Aspects of Integral Optics*. Moscow: MIEM (1983) 130pp; Journal version in: *Russ. J. Math. Phys.* 8 (2001) 83–105 and 180–238.
40. N.S. Bakhvalov and G.P. Panasenko, *Homogenization: Averaging Processes in Periodic Media. Mathematical Problems in the Mechanics of Composite Materials*. Moscow: Nauka (1984) 352pp; N.S. Bakhvalov and G.P. Panasenko, *Homogenization: Averaging Processes in Periodic Media. Mathematical Problems in the Mechanics of Composite Materials*. In: *Mathematics and Its Applications: Soviet Series* 36. Dordrecht etc.: Kluwer Academic Publishers (1989) xxxv+366pp.
41. V.G. Vaks, *Interatomic Interactions and Bonds in Solids*. (in Russian). Moscow: IzdAT (2002) 256pp.
42. M.I. Katsnelson and A.V. Trefilov, *Crystal Lattice Dynamics and Thermodynamics*. (in Russian). Moscow: IzdAT (2002) 382pp.
43. V.S. Buslaev, Quasiclassical approximation for equations with periodic coefficients. *Uspekhi Mat. Nauk* 42 (1987) 77–98; V.S. Buslaev, Quasiclassical approximation for equations with periodic coefficients. *Russ. Math. Surveys* 42 (1987) 97–125.
44. V.S. Buslaev, Adiabatic perturbation of a periodic potential. (in Russian). *Teor. Mat. Fiz.* 58 (1984) 223–243.
45. A. Fedotov and F. Klopp, Anderson transition for a family of almost periodic Schrödinger equations in the adiabatic case. *Comm. Math. Phys.* 227 (2002) 1–92.
46. S.Yu. Dobrokhotov, Resonances in asymptotic of a solution of the Cauchy problem for the Schrödinger equation with a rapidly oscillating finite-zone potential. *Mat. Zametki* 44 (1988) 319–340; S.Yu. Dobrokhotov, Resonances in asymptotic of a solution of the Cauchy problem for the Schrödinger equation with a rapidly oscillating finite-zone potential. *Math. Notes* 44 (1988) 1015–1033.
47. E.I. Blount, Bloch electrons in a magnetic field. *Phys. Rev.* 126, 5 (1961) 1636–1653.
48. S.P. Novikov and A.Ya. Maltsev, Topological phenomena in normal metals. *Usp. Fiz. Nauk* 168 (1998) 249–258; S.P. Novikov and A.Ya. Maltsev, Topological Phenomena in Normal Metals. *Phys. – Usp.* 41 (1998) 231–239.
49. W.P. Su, I.R. Schrieffer and A.J. Heeger, Soliton excitations in polyacetylene. *Phys. Rev. B* 22 (1980) 2099–2111.
50. J.M. Ziman, *Principles of the Theory of Solids*. Cambridge: Cambridge University Press (1964) xiii+360pp.
51. S.A. Brazovskii, I.E. Dzyaloshinskii and I.M. Krichever, Exactly soluble Peierls models. *Zh. Exper. Teor. Fiz.* 83 (1982) 389–404; S.A. Brazovskii, I.E. Dzyaloshinskii and I.M. Krichever, Exactly soluble Peierls models. *Phys. Lett. A* 83 (1982) 40–42.
52. I.M. Krichever, Algebraic curves and non-linear difference equations. *Usp. Mat. Nauk* 33 (1978) 215–216; I.M. Krichever, Algebraic curves and non-linear difference equations. *Russ. Math. Surveys* 33 (1978) 255–256.
53. S.Yu. Dobrokhotov and Yu.M. Vorob'ev, Semiclassical asymptotics for discrete models of electron-phonon interaction. *Teor. Mat. Fiz.* 57 (1983) 63–74; S.Yu. Dobrokhotov and Yu.M. Vorob'ev, Semiclassical asymptotics for discrete models of electron-phonon interaction. *Theor. Math. Phys.* 57 (1983) 993–1001.
54. S.I. Badulin, V.I. Shrira and L.Sh. Tsimring, The trapping and vertical focusing of internal waves in a pycnocline due to the horizontal inhomogeneities of density and currents. *J. Fluid Mech.* 158 (1985) 199–218.
55. V.P. Maslov, Asymptotics of eigenfunctions of the equation  $\Delta u + k^2 u = 0$  with boundary conditions on equidistant curves and the scattering of electromagnetic waves in a waveguide. (in Russian). *Dokl. Akad. Nauk SSSR* 123 (1958) 631–633.
56. E.M. Vorob'ev and V.P. Maslov, On the Single-mode open resonators. (in Russian). *Dokl. Akad. Nauk SSSR* 179 (1968) 558–561.
57. P. Exner, A quantum pipette. *J. Phys. A: Math. Gen.* 28 (1995) 5323–5330.

58. K. Lin and R.L. Jaffe, Bound states and threshold resonances in quantum wires with circular bends. *Phys. Rev. B* 54 (1996) 5750–5762.
59. G.F. Dell’Antonio and L. Tenuta, Semiclassical analysis of constrained quantum systems. *J. Phys. A: Math. Gen.* 37 (2004) 5605–5624.
60. A.G. Voronovich, The propagation of surface and internal gravitational waves in approximation of geometric optics. (in Russian). *Izv. Akad. Nauk SSSR. Ser. Fizika Atmosfery i Okeana* 12 (1976) 850–857.
61. S.Yu. Dobrokhotov, P.N. Zhevandrov, A.A. Korobkin and I.V. Sturova, Asymptotic theory of propagation of nonstationary surface and internal waves over uneven bottom. In: K.-H. Hoffmann and D. Mittelmann (eds.), *International Series of Numerical Mathematics* 106. Basel, Berlin etc.: Birkhäuser Verlag (1992) pp.105–112.
62. J. Brüning, S.Yu. Dobrokhotov, R.V. Nekrasov and T.Ya. Tudorovskiy, Quantum and classical dynamics of an electron in 2144 thin film. To appear in *Russ. J. Math. Phys.*
63. S. Iijima, Helical microtubules of graphitic carbon. *Nature* 354 (1991) 56–58.
64. R. Saito, G. Dresselhaus and M.S. Dresselhaus, *Physical Properties of Carbon Nanotubes*. London: Imperial College Press (1998) xii + 259 pp.
65. Ph. Avouris, T. Hertel, R. Martel, T. Schmidt, H.R. Shea and R.E. Walkup, Carbon Nanotubes: nanomechanics, manipulation and electronic devices. *Appl. Surf. Sci.* 141 (1999) 201–209.
66. L.A. Chernozatonskii, E.G. Gal’pern, N.R. Serebryanaya and I.V. Stankevich, Polymers of single-wall nanotubes: geometry, diffraction patterns, and electronic spectrum modeling. In: H. Kuzmany, J. Fink, M. Mehring and S. Roth. (eds.), *AIP Conf. Proc.* 486. Melville, New York: American Institute of Physics (1999) pp.284–305.
67. I.V. Stankevich, Diversity of carbon forms: hypothesis and reality. *Mol. Mat.* 7 (1996) 1–12.
68. A.V. Eletsii, Carbon nanotubes. *Usp. Fiz. Nauk* 167 (1997) 945–972; A.V. Eletsii, Carbon nanotubes. *Phys. – Usp.* 40 (1997) 899–924.
69. A.V. Eletsii, Carbon nanotubes and their emission properties. *Usp. Fiz. Nauk* 172 (2002) 401–438; A.V. Eletsii, Carbon nanotubes and their emission properties. *Phys. – Usp.* 45 (2002) 369–402.
70. V.Ya. Prinz, D. Grützmacher, A. Beyer, C. David, B. Ketterer and E. Deckardt, A new technique for fabricating three-dimensional micro- and nanostructures of various shapes. *Nanotechnology* 12 (2001) 399–402.
71. V. Gantmakher and Y. Levinson, *Carrier Scattering in Metals and Semiconductors*. Moscow: Nauka (1984) 350 pp; V. Gantmakher and Y. Levinson, *Carrier Scattering in Metals and Semiconductors*. In: V.M. Agranovich and A.A. Maradudin (eds.), *Modern Problems in Condensed Matter Science* 19. Amsterdam: North-Holland Publishing Co. (1987) xviii + 478 pp.
72. V.V. Belov, S.Yu. Dobrokhotov and S.O. Sinitsyn, Asymptotic solutions of the Schrödinger equation in thin tubes. *Trudy Instituta Matematiki i Mehaniki UrO RAN* 9 (2003) 1–11; V.V. Belov, S.Yu. Dobrokhotov and S.O. Sinitsyn, Asymptotic solutions of the Schrödinger equation in thin tubes. *Proc. Steklov Inst. Math.*, suppl. 1 (2003) S13–S23.
73. V.V. Belov, S.Yu. Dobrokhotov, S.O. Sinitsyn and T.Ya. Tudorovskii, Quasiclassical approximation and the Maslov canonical operator for nonrelativistic equations of quantum mechanics in nanotubes. *Dokl. Akad. Nauk. Ser. Mat.* 393 (2003) 460–464; V.V. Belov, S.Yu. Dobrokhotov, S.O. Sinitsyn and T.Ya. Tudorovskii, Quasiclassical approximation and the Maslov canonical operator for nonrelativistic equations of quantum mechanics in nanotubes. *Dokl. Math. Ser. Math. Phys.* 68 (2003) 460–465.
74. V.V. Belov, S.Yu. Dobrokhotov and T.Ya. Tudorovskii, Quantum and classical dynamics of an electron in thin curved tubes with spin and external electromagnetic fields taken into account. *Russ. J. Math. Phys.* 11 (2004) 109–119.
75. V.M. Babich and V.S. Buldyrev, *Asymptotic Methods in Short Wave Diffraction Problems. Method of Etalon Problems*. Moscow: Nauka (1972) 456 pp; V.M. Babich and V.S. Buldyrev, *Short-Wavelength Diffraction Theory: Asymptotic Methods*. In: H.K.V. Lotsch (ed.-in-chief), L.M. Brekhovskikh, L.B. Felsen and H.A. Haus (eds.), *Springer Series on Wave Phenomena* 4. Berlin etc.: Springer-Verlag (1991), xi + 445 pp.
76. P.K. Rashevskii, *Riemannian Geometry and Tensor Analysis*. Moscow: Nauka (1967) 664 pp; P.K. Rashevskii, *Riemann’sche Geometrie und Tensoranalysis*. Berlin: Deutscher Verlag der Wissenschaften (1959) 606 pp.
77. V.V. Kucherenko, Asymptotics of solution of the system  $A(x, -i\hbar\partial_x)u=0$  as  $\hbar\rightarrow 0$  in the case of characteristics of variable multiplicity. (in Russian). *Izv. Akad. Nauk SSSR. Ser. Mat.* 38 (1974) 625–662.
78. A. Gordon and J. E. Avron, Born-Oppenheimer approximation near level crossing. *Phys. Rev. Lett.* 85 (2000) 34–37.
79. J.E. Avron and A. Gordon, Born-Oppenheimer wave function near level crossing. *Phys. Rev. A* 62 (2000) 062504-1–062504-9.

80. Y. Colin de Verdière and B. Parisse, Singular Bohr-Sommerfeld rules. *Comm. Math. Phys.* 205 (1999) 459–500.
81. T. Hertel, R.E. Walkup and P. Avouris, Deformation of carbon nanotubes by surface van der Waals forces. *Phys. Rev. B* 58 (1998) 13870–13873.
82. A.S. Davydov, *Quantum Mechanics*. Moscow: Fizmatgiz (1963) 748 pp; A.S. Davydov, *Quantum Mechanics*. In: *International Series of Monographs in Natural Philosophy* 1. Oxford, London, Edinburgh: Pergamon Press (1965) xiii+680 pp.
83. B.R. Vainberg, *Asymptotic Methods in Equations of Mathematical Physics*. Moscow: Moscow University Publ. (1982) 293 pp; B.R. Vainberg, *Asymptotic Methods in Equations of Mathematical Physics*. New York etc.: Gordon and Breach Science Publishers (1989) vii+498 pp.
84. V.V. Belov, S.Yu. Dobrokhotov and T.Ya. Tudorovskiy, Asymptotic solutions of nonrelativistic equations of quantum mechanics in curved nanotubes. I. Reduction to spatially one-dimensional equations. *Teor. Mat. Fiz.* 141 (2004) 267–303; V.V. Belov, S.Yu. Dobrokhotov and T.Ya. Tudorovskiy, Asymptotic solutions of nonrelativistic equations of quantum mechanics in curved nanotubes. I. Reduction to spatially one-dimensional equations. *Theor. Math. Phys.* 141 (2004) 1562–1592.
85. T.Ya. Tudorovskiy, On the Effect of Spin on Classical and Quantum Dynamics of an Electron in Thin Twisted Tubes, *Mathematical Notes*, vol. 78, no. 6, 2005, pp. 883–889. Translated from *Matematicheskii Zametki*, vol. 78, no. 6, 2005, pp. 948–953.
86. A. Bensoussan, G.L. Lions and G.C. Papanicolaou, *Asymptotic Analysis for Periodic structures*. In: *Studies in Mathematics and its Applications* 5. Amsterdam: North-Holland Publishing Co. (1978) xxiv+700 pp.
87. V.A. Marchenko and E.Ya. Khruslov, *Boundary-Value Problems in Domains with Fine-Grained Boundary*. (in Russian). Kiev: Naukova Dumka (1974) 279 pp.
88. V.V. Jikov, S.M. Kozlov and O.A. Oleĭnik, *Homogenization of Differential Operators and Integral Functionals*. Berlin etc.: Springer-Verlag (1994) xi+570 pp.
89. V.A. Geiler and I.Yu. Popov, Ballistic transport in nanostructures: explicitly solvable model. *Teor. Mat. Fiz.* 107 (1996) 12–20; V.A. Geiler and I.Yu. Popov, Ballistic transport in nanostructures: explicitly solvable model. *Theor. Math. Phys.* 107 (1996) 427–434.
90. V.P. Maslov and M.V. Fedoryuk, *Quasiclassical Approximation for the Equations of Quantum Mechanics*. Moscow: Nauka (1976) 296 pp; V.P. Maslov and M.V. Fedoryuk, *Semi-Classical Approximation in Quantum Mechanics*. In: *Mathematical Physics and Applied Mathematics* 7, *Contemporary Mathematics* 5. Dordrecht etc.: D. Reidel Publishing Co. (1981) ix+301 pp.
91. J. Brüning, S.Yu. Dobrokhotov and K.V. Pankrashkin, The spectral asymptotics of the two-dimensional Schrödinger operator with a strong magnetic field. *Russ. J. Math. Phys.* 9 (2002) 14–49 and 400–416.
92. N.A. Poklonski, E.F. Kislyakov, G.G. Fedoruk and S.A. Vyrko, Electronic structure model of a metal-filled carbon nanotube. *Fiz. Tverd. Tela* 42 (2000) 1911–1916; N.A. Poklonski, E.F. Kislyakov, G.G. Fedoruk and S.A. Vyrko, Electronic structure model of a metal-filled carbon nanotube. *Phys. Solid State* 42 (2000) 1966–1971.
93. S.G. Lemay, J.W. Janssen, M. van den Hout, M. Mooij, M.J. Bronikowski, P.A. Willis, R.E. Smalley, L.P. Kouwenhoven and C. Dekker, Two-dimensional imaging of electronic wavefunctions in carbon nanotubes. *Nature* 412 (2001) 617–620.